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US High Production Volume Chemical Program

**Category Summary
For
High Benzene Naphthas Category**

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**Prepared by:
Olefins Panel of the American Chemistry Council**

December 10, 2004

EXECUTIVE SUMMARY

The Olefins Panel of the American Chemistry Council (ACC) hereby submits the category summary report for the High Benzene Naphthas Category under the U.S. Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program. The purpose of this report is to:

- Present results of an assessment to determine whether the 19 CAS numbers which represent 10 production streams are adequately characterized with the existing data from hydrocarbon constituents of the production streams and analogous mixtures as described in the High Benzene Naphthas Category test plan.
- Summarize the SIDS (Screening Information Data Set) physicochemical, environmental fate and effects, and human health HPV program endpoints for the High Benzene Naphthas Category.
- Provide a description of manufacturing processes, potential exposure sources, and uses for High Benzene Naphtha streams.
- Demonstrate that the extensive body of data available for mammalian and environmental endpoints on representative constituents of products in this category, and streams of similar complex hydrocarbon composition, as well as some data on representative streams within the category are sufficient to fully define the High Benzene Naphthas Category.

The High Benzene Naphthas Category is composed of 10 ethylene manufacturing streams that exhibit commonalities of manufacturing process and composition. The 19 CAS numbers in this category each represent at least one of the category production streams. In some cases, a single CAS number represents more than one stream. The production streams consist of complex hydrocarbon reaction products, predominantly C5 through C11, through components boiling at 650°F or higher, and may be correctly represented by more than one CAS number.

Pyrolysis gasoline is the major stream in this category and essentially all of the other category streams are derived from it, either as simple distillate fractions or hydrogenated distillate fractions. These streams all contain significant concentrations of benzene, generally greater than 10% and averaging 55%. They are the industry's intermediate streams that are processed to high purity benzene and other by-products. Pyrolysis gasoline and these fractions account for 99.9% of the category production. The remaining 0.1% of the category production consists of similar benzene-containing industry streams.

Exposure

The primary use of streams in the High Benzene Naphthas Category is the isolation of high purity benzene. There are no known consumer uses for these category streams. The streams are either used on the site where they were produced or shipped to other industrial sites for additional processing. Production is performed in closed systems and products are transported in bulk in closed systems by pipeline, barge, tank car or tank truck. The streams are typically inventoried in bulk storage tanks, either floating roof or fixed roof with vents routed to a control device in order to reduce emissions. Environmental exposure can occur through accidental spills, fugitive emissions, leakage or release of vapors into the atmosphere during tankage, delivery, or transfer for storage.

Exposure of workers is expected to be minimal because high benzene naphtha streams are isolated in production or used in closed system process units. Exposure could occur by inhalation of low-level concentrations of fugitive emissions from process units or storage tanks, from sampling, or by displaced emissions during loading of bulk transportation vessels, from emissions from control devices such as flares, or dermally by accidental spillage. The general population is not usually exposed to high benzene naphthas unless situated near industrial facilities that use or produce the category streams, but may be exposed to benzene through inhalation of contaminated ambient air, particularly in heavy traffic areas and around filling stations or in cigarette smoke-filled environments. The OSHA Benzene Standard applies to streams in the High Benzene Naphthas Category and limits occupational exposure. OSHA and ACGIH have established guidelines for other components (e.g. toluene, pentane, naphthalene, styrene) found in the category streams.

Human Health

Evaluation of data on representative streams and read-across from chemical components indicate that High Benzene Naphtha streams are not acutely toxic by the oral, dermal or inhalation routes of exposure. Data suggests that it is unlikely that most streams in this category would cause significant genetic toxicity. Tested streams did not cause mutational events in bacteria, and a weak direct effect in mammalian cells from treatment with a C5-C10 fraction of Pyrolysis gasoline was not confirmed *in vivo* by any expression of gene mutation in *Drosophila*. Although these streams contain substantial concentrations of benzene, a known clastogen, no cytogenetic damage was induced by oral treatment of rats with the Hydrogenated C6-C8 stream [55% benzene], demonstrating the inhibitory effects of other components in the stream, probably from competition for metabolic sites.

Benzene, as a predominant component in most streams is considered a key driver in establishing health effects within the SIDS battery of tests. To provide a conservative estimate of health hazard, results of benzene-induced systemic toxicity must be addressed – hazards from components should be considered hazards for the streams until sufficient data become available to show the specific combination of components does not present a hazard. However, as it has been demonstrated in the area of cytogenetics, the presence of biologically active components blended together can inhibit toxicity inducible by individual components. Repeated dose studies from 2 representative streams in the category reported skin irritation and concomitant effect on dermal tissue histologically [NOAEL<0.10ml/kg] but no other systemic toxicity in rabbits, and lethargy and labored respiration in rats from inhalation exposure at high doses [NOAEL<4869ppm]. Results were similar to effects reported in the API Gasoline Blending Streams test plan, effects from which animals recovered after 4 weeks without exposure. Such data suggest that toxicity of the blended streams may be less severe than that of individual components due to lower individual component concentrations, component interaction and competitive inhibition. No significant reproductive effects were reported in multi-generation studies of stream components. Developmental effects from components present in High Benzene Naphtha streams occurred primarily at doses that were maternally toxic as well. A developmental study in rabbits with a representative high benzene naphtha stream did not result in adverse effects on any developmental parameters except for 1 high dose rabbit that aborted, and no malformations were induced [NOAEL = 50mg/kg].

Environmental

For environmental endpoints, measured data on components present in the products of the High Benzene Naphthas Category, and on other complex products that contain a similar range of chemical classes and carbon numbers were used. These data demonstrate that the hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric

oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 0.9 - 65.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modeling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data show that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates. Aquatic toxicity for products in this category can be predicted based on carbon number, measured or calculated toxicities of constituent hydrocarbons and constituent composition.

Conclusions

The data available for mammalian and environmental endpoints on representative constituents of products in this category, and streams of similar complex hydrocarbon composition and on some data from representative streams, are sufficient to characterize the potential toxicity for streams in this category and demonstrate the integrity of the category, itself, for purposes of the HPV Program.

New data on hydrocarbons present in High Benzene Naphtha streams that are developed in other HPV programs will be evaluated when they become available in the context of the present completed assessment. This category summary document will be amended should the new data result in substantial changes to the conclusions.

AMERICAN CHEMISTRY COUNCIL

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*Companies that are part of the Panel but do not produce products in the
High Benzene Naphthas Category

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1 CATEGORY DESCRIPTION AND JUSTIFICATION

1.1 Category Identification

The High Benzene Naphthas Category was developed for the HPV program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The 19 CAS numbers listed in Table 1 describe 10 streams which are complex products containing many components. Certain single streams are correctly represented by more than one CAS number, and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix 1.

The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher.

The CAS Numbers in the High Benzene Naphthas Category are associated with the following streams, which are commercial products or isolated intermediates:

Pyrolysis Gasoline
Pyrolysis C6 Fraction
Pyrolysis C6-C8 Fraction
Pyrolysis C5-C6 Fraction
Hydrotreated C6 Fraction
Hydrotreated C6-C7 Fraction
Hydrotreated C6-C8 Fraction
Quench Loop Pyrolysis Oil and Compressor Oil
Recovered Oil from wastewater treatment
Aromatic Extract from Benzene Extraction

Pyrolysis gasoline, is the major product in this category. Pyrolysis gasoline and its 3 distillate fractions together make up about 66% of the production capacity in the category. Test data exists for one of these 4 streams (pyrolysis gasoline) and for a fraction of pyrolysis gasoline. Three hydrotreated pyrolysis gasoline fractions make up approximately 33% of the production capacity in the category and test data exist for one of these 3 streams. The remaining 3 streams are included in this category because they are similar benzene-containing intermediate streams produced by industry.

Table 1. CAS Numbers¹ and CAS Names Associated with Streams in the High Benzene Naphthas HPV Category

Production Streams	CAS RN	CAS RN Name
Pyrolysis Gasoline	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
	68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. residues
	64742-83-2	Naphtha, petroleum, light steam-cracked
	64742-91-2	Distillates, petroleum, steam-cracked
	67891-79-6	Distillates, petroleum, heavy arom.
	67891-80-9	Distillates, petroleum, light arom.
	68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
	68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
	68606-28-0	Hydrocarbons, C5 and C10-aliph. and C6-8-arom.
	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
Pyrolysis C5-C6 Fraction	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68956-52-5	Hydrocarbons, C4-8
Pyrolysis C6 Fraction	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
Pyrolysis C6-C8 Fraction	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
	64742-83-2	Naphtha, petroleum, light steam-cracked
	68476-45-9	Hydrocarbons, C5-10 arom. conc., ethylene-manuf.-by-product
Hydrotreated C6 Fraction	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
	8030-30-6	Naphtha
Hydrotreated C6-C7 Fraction	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
	64742-49-0	Naphtha, petroleum, hydrotreated light
	64742-73-0	Naphtha, petroleum, hydrodesulfurized light
	68955-29-3	Distillates, petroleum, light thermal cracked, debutanized arom.
Hydrotreated C6-C8 Fraction	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
Quench Loop Pyrolysis Oil and Compressor Oil	69013-21-4	Fuel oil, pyrolysis
Recovered Oil from Wastewater Treatment	68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
Aromatic Extract from Benzene Extraction	64741-99-7	Extracts, petroleum, light naphtha solvent

Note 1: The CAS numbers associated with the corresponding production streams are shown in the above table. In some cases, more than one CAS number is used to represent a specific stream and in other cases a single CAS number may be used to represent more than one stream. The Olefins Industry or others may use these same CAS numbers to represent substances that may, in various degrees, be dissimilar to the category streams. CAS numbers, other than those shown in this table may be used to describe these streams in future reporting.

Descriptions of the 10 streams associated with the High Benzene Naphthas Category are presented below:

1. Pyrolysis Gasoline

Pyrolysis Gasoline (Pygas) consists predominantly of C5+ hydrocarbons produced by ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the

debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinyl acetate at a concentration of up to about 10%. Vinyl acetate is not typically found in ethylene process streams.

2. Pyrolysis Gasoline Fractions

Pyrolysis gasoline is separated by distillation into various boiling-point-range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this separation.

(a) Pyrolysis C5-C6 Fraction

The carbon number distribution for this stream is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

(b) Pyrolysis C6 Fraction

The carbon number distribution for this stream is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

(c) Pyrolysis C6-C8 Fraction

This stream has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

3. Hydrotreated Pyrolysis Fractions

Pyrolysis gasoline or distillate fractions of pyrolysis gasoline are sometimes treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformat fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics into alkyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained

olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.

(a) Hydrotreated C6 Fraction

This stream is very similar in composition to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%.

(b) Hydrotreated C6-C7 Fraction

The carbon number distribution for this stream is predominantly C6 -C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.

(c) Hydrotreated C6-C8 Fraction

The reported typical compositions for this stream are 40 to 60% benzene, 10 to 25% toluene and 3 to 10% C8 aromatics.

4. Quench Loop Pyrolysis Oil and Compressor Oil

Quench Loop Pyrolysis Oil (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene.

5. Recovered Oil from Wastewater Treatment

This stream can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information have been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

6. Aromatic Extract from Benzene Extraction

Hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered as the Aromatic Extract from Benzene Extraction. The carbon number

distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

1.2 Purity/Impurities/Additives

CAS numbers in this category are used to represent extremely complex mixture of hydrocarbons in the C5 – C11 carbon range. Typically there are no impurities in the streams in this category. The typical compositions of streams in this category are listed in Appendix 2 Table A2-1 and Figures 4 and 5.

1.3 Physico-Chemical Properties

Properties for the High Benzene Naphthas category have been estimated from calculated and measured values for representative constituents of the category. Substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent physico-chemical properties of the category are C5 –C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Calculated data have been derived using subroutines of the EPIWIN© version 3.04 computer model (EPIWIN, 1999) described in the US EPA document “The Use of Structure-Activity Relations (SAR) in the High Production Volume Chemical Challenge Program (US EPA, 1999).” Robust summaries for Physico-Chemical property studies are provided as Attachment 1a.

Table 2. Summary of Calculated Physico-Chemical Properties for Selected Chemicals Contained by Streams in the High Benzene Naphthas Category

Substance Constituent	Melting Point (°C)	Boiling Point (°C@760mm Hg)	Vapor Pressure (hPa@ 25°C)	Log K _{ow} (@ 25°C)	Water Solubility (mg/L@25°C)
Isoprene	-118.89	34.95	7.35 E ²	2.58	247.2
n-pentane	-106.92	46.01	6.84 E ²	2.80	159.7
1,3-cyclopentadiene	-91.83	69.17	5.69 E ²	2.25	470.6
Isohexane	-105.80	56.26	2.48 E ²	3.21	66.94
n-hexane	-93.84	71.53	2.00 E ²	3.29	57.42
Methylcyclopentane	-85.82	80.34	1.77 E ²	3.10	83.95
Benzene	-77.92	102.24	1.16 E ²	1.99	2634.0
Toluene	-59.17	125.72	31.60	2.54	832.7
m-Xylene	-40.69	148.29	8.83	3.09	258.4
Styrene	-48.31	146.65	6.73	2.89	386.7
Dicyclopentadiene	-16.78	176.78	2.20	3.16	na
Naphthalene	5.01	231.64	0.05	3.17	142.1

na =not available.

Calculated values determined by EPIWIN [EPIWIN 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.].

Table 3. Summary of Measured Physico-Chemical Properties for Selected Chemicals Contained by Streams in the High Benzene Naphthas Category

Substance Constituent	Melting Point (°C)	Boiling Point (°C@760mm Hg)	Vapor Pressure (hPa @ 25°C)	Log K _{ow} (@ 25°C)	Water Solubility (mg/L@25°C)
Isoprene	-145.9	34.0	7.33 E ²	2.42	338.6
n-pentane	-129.7	36.0	6.85 E ²	3.39	49.8
1,3-cyclopentadiene	- 85.0	41.0	5.80 E ²	na	na
Isohexane	-162.9	63.2	2.53 E ²	3.60	31.1
n-hexane	- 95.3	68.7	2.01 E ²	3.90	17.2
Methylcyclopentane	-142.5	71.8	1.84 E ²	3.37	49.4
Benzene	5.5	80.0	1.26 E ²	2.13	2000.0
Toluene	- 94.9	110.6	37.86	2.73	573.1
m-Xylene	- 47.8	139.1	11.05	3.20	207.2
Styrene	- 31.0	145.0	8.53	2.95	343.7
Dicyclopentadiene	32.0	170.0	3.05	na	na
Naphthalene	80.2	217.9	0.11	3.30	142.1

na = not available

Measured values from the experimental database in EPIWIN [EPIWIN, 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.].

The following ranges can be used to define the five physico-chemical endpoints of substances in this category. The calculated and measured ranges overall compare favorably with each other.

1.3.1 Melting Point (Range)

The calculated melting points (by subroutine MPBPWIN, version 1.40) for representative constituents that are present in the category streams vary from -118.89 to 5.01°C. The measured melting points of these same constituents vary from -162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside these ranges may be possible for some category streams.

1.3.2 Boiling Point (Range)

The calculated boiling points (by subroutine MPBPWIN, version 1.40) for representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside these ranges may be possible for some category streams.

1.3.3 Vapor Pressure (Range)

The calculated vapor pressures (by subroutine MPBPWIN, version 1.40) for representative constituents that are present in the category streams vary from 0.05 to 7.35 E² hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 E² hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside these ranges may be possible for some category streams.

1.3.4 Partition Coefficient: Log K_{ow} (Range)

The calculated log K_{ow} (by subroutine KOWWIN, version 1.65) for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.13 to 3.90 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside these ranges may be possible for some category streams.

1.3.5 Water Solubility (Range)

The calculated water solubility (by subroutine WSKOWWIN, version 1.36) for some representative constituents that are present in the category streams vary from 57.42 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside these ranges may be possible for some category streams.

1.4 Category Justification

The High Benzene Naphthas Category is comprised of 10 streams associated with 19 CAS numbers, which are complex products containing high levels of benzene (10-80%) plus many other components (predominantly C5-C11), many of which are shared across streams. The average benzene content is 55%. All streams in this category are subject to the Occupational Safety and Health Administration (OSHA) Benzene Standard (29 CFR 1910.1028). Those streams containing 1,3-butadiene are subject to the OSHA Butadiene Standard (29 CFR 1910.1051). OSHA Permissible Exposure Limits exist for most major components. Benzene, as the predominant component in most streams, is expected to be the key driver with respect to health effects endpoints within the SIDS battery of tests, with genotoxicity and hematotoxicity the effects most likely to be seen. However, the other components may also contribute to the toxicity of the streams. Pyrolysis gasoline is the major stream in this category and essentially all of the other category streams are derived from it, either as simple distillate fractions or hydrogenated distillate fractions. They are the Olefins Industry's intermediate streams that are processed to high purity benzene and other byproducts. Pyrolysis gasoline and these fractions account for 99.9% of the category production. The remaining 0.1% of the category production consists of similar benzene-containing industry streams.

The basic strategy of this screening level test plan for characterizing the human health hazards of this category is to evaluate data for representative streams in the category, for the components of the streams, as well as data for mixtures of category components and analogous mixtures.

Benzene has a robust toxicity dataset, including data on human experience, and has completed the OECD SIDS program. The existing epidemiology and toxicology database for the components other than benzene and for mixtures containing the components is extensive. All components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for their structural analogs.

Additional data for the components, or for structural analogs of components, are under development by the American Chemistry Council Olefins Panel for other categories under the HPV program (Appendix 7), by other HPV consortia, and by the OECD SIDS program (Appendix 3, Table A3-1). Furthermore, some of the materials obtained by distillation from Pyrolysis Gasoline are being tested in other Panel HPV Test Plans (Non-Cyclic C5s and Resin Oils and Cyclodiene Dimer Concentrates categories); and the High Benzene Naphthas Category shares many of the same components with the gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan. These gasoline stream data can contribute to the hazard evaluation for the members of this category by showing effects, or lack thereof, due to mixtures containing components of this category when the benzene content is very low (~ 2%).

For the HPV program, the Panel believes that the human health hazards of the category can be adequately characterized by using scientific judgment to analyze component data (existing data and data being developed by other testing programs), without conducting additional toxicology tests. The Panel further believes that additional testing on streams is unlikely to demonstrate any adverse effects that have not been shown for components, and would provide little useful data for regulatory, industrial hygiene, emergency response or hazard communication purposes.

Assessment of human health hazards for category members has been developed using data from testing of representative streams, and data from the sources listed in Appendix 4. Assessments will be supplemented and revised, if needed, as data becomes available for other cited testing programs now in progress.

The strategy for characterizing the physical-chemical properties, and environmental hazards of products in the High Benzene Naphthas Category also employs a constituent approach, evaluating measured data on high purity hydrocarbons and components of reaction products in the High Benzene Naphthas Category. Where measured data do not exist, calculated data for selected constituents of these naphthas have been developed using the Epiwin© computer models described by EPA. For biodegradability and aquatic toxicity, data on component chemicals contained in streams in this category and similar complex products were evaluated and read-across assessments developed.

2 EXPOSURE AND USE

The Category and HPV Stream Production:

The High Benzene Naphthas Category includes ten product streams produced by the Olefins Processes. The category streams are complex mixtures with variable compositions and all contain significant concentrations of benzene. Benzene is separated from the category streams, or from streams obtained from the category streams, in downstream processing units. The category streams are isolated intermediates that are used on site where they are manufactured or transferred under controlled conditions to a limited number of locations within the same company or to second parties that use the streams in a controlled way as an intermediate with well-known technology.

Pyrolysis gasoline is the primary stream in the category. This stream is produced by the ethylene production process and consists of a complex mixture of hydrocarbons, primarily carbon number 5 and higher. Typically, Pyrolysis Gasoline contains about 40% benzene, although the content reported for this program varied from 15% to 62%. Pyrolysis gasoline is separated by distillation into various boiling-point-range streams. Some of these streams are included in this HPV category, and some in other categories of the Olefins Panel's HPV program. Typically, the Pyrolysis Gasoline-derived streams include a C5 fraction (Olefins Panel HPV C5 non-Cyclics); various benzene-containing fractions (streams in this HPV category); non-benzene, gasoline-like streams (Olefins Panel HPV Low Benzene Naphthas); aromatic or aromatic/cyclodiene dimer streams (Olefins Panel HPV Resin Oils & Cyclodiene Dimer Concentrates); and fuel oil streams (Olefins Panel HPV Fuel Oils). Pyrolysis Gasoline, or intermediate streams derived from pyrolysis gasoline are typically hydrogenated, which is a necessary processing step prior to isolation of benzene by extraction or extractive distillation. The hydrogenation step produces the hydrogenated streams in this HPV category as well as in the hydrogenated streams in the Olefins Panels HPV C5 non-Cyclics and HPV Low Benzene Naphthas categories. Distribution of the 24 billion pounds/year¹ of category production among the category streams is shown in Figure 1.

Combustion processes and other industrial processes also produce the individual hydrocarbon components present in the complex streams of the category. Potential exposures to these individual components from other manufacturing processes, from combustion, or from natural sources are considered to be out of scope for this assessment. This assessment is limited to potential exposures to the streams in the category. Some data are presented for specific components of the category streams, which is intended to help clarify the potential for exposure to the streams. There are nineteen CAS numbers that are used by the Olefins Industry to represent the ten category streams. This assessment addresses the use of these CAS numbers for the High Benzene Naphtha Category streams. Some of the CAS numbers in this category may be used by the Olefins Industry or others to represent other substances that are not included in the High Benzene Naphthas Category, and may be included in other HPV categories.

This screening level exposure assessment is based on information received from fourteen of the sixteen original sponsors of the category and upon other available information.

¹ 24 Billion pounds per year is the approximate total annual commercial production of category streams reported by the sponsors of the category and based on their 1998 TSCA IUR.

Figure 1
High Benzene Naphthas
Category Production (1998 Data)

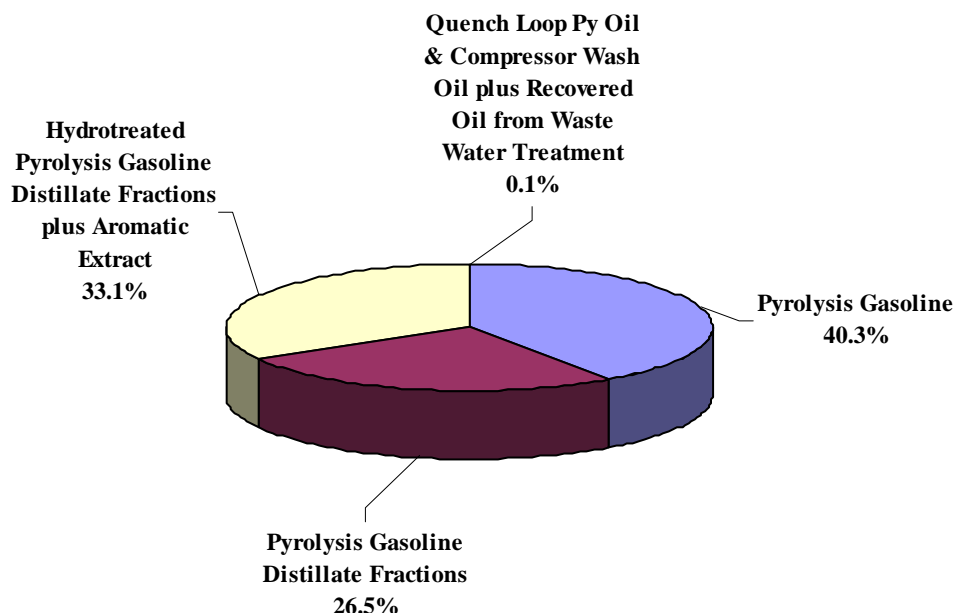


Table 4. High Benzene Naphthas Category Streams

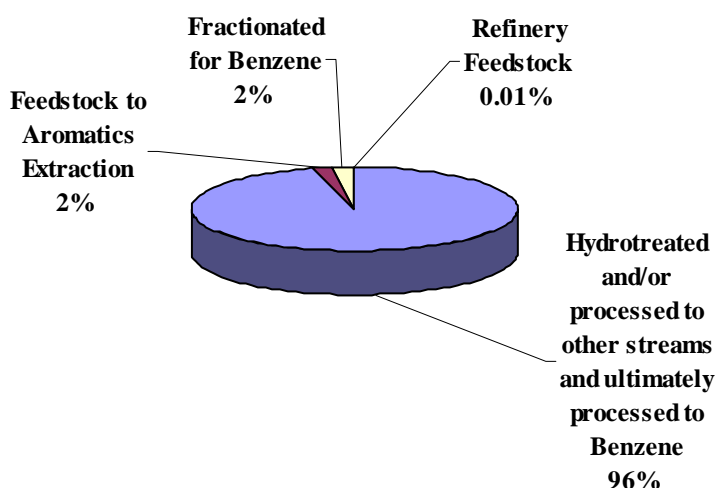
Pyrolysis Gasoline & Distillate Fractions	Hydrotreated Fractions & Aromatic Extract	Other Category Streams
Pyrolysis Gasoline	Hydrotreated C6-C7	Recovered Oil from Waste Water Treatment
Pyrolysis C6	Hydrotreated C6-C8	Quench Loop Pyrolysis Oil & Compressor Wash Oil
Pyrolysis C6-C8	Hydrotreated C6	
Pyrolysis C5-C6	Aromatic Extract from Benzene Extraction	

Storage and Transportation of Category Streams: The High Benzene Naphtha streams are either used on-site where they were produced, or shipped to other industrial sites for additional processing. When shipped between industrial sites, the category streams are transported in bulk in closed systems by pipeline, barge, tank car or tank truck. The streams are typically inventoried in bulk storage tanks, either floating roof or fixed roof with vents routed to a control device in order to reduce emissions.

Use: There are no known consumer uses for these category streams. Uses of the category streams are shown in Figure 2. Pyrolysis Gasoline and other category intermediates streams are processed to produce other streams in this category or streams in other of the Olefins Panel's

HPV categories, as discussed above. Figure 2 illustrates that 96% of the category volume is processed to benzene and other intermediate streams, most of which are not isolated intermediates in this HPV category. Only 4% of the category volume is isolated from the process prior to being transferred to the aromatic extraction unit (for benzene production) or transferred to the Benzene fractionation unit. Virtually all of the benzene contained in the category streams is ultimately isolated as high purity benzene product, which is the primary use of the category streams. Some of the non-benzene components of the streams are isolated as other streams. Figure 2 does not include use data for the following three category streams – Recovered Oil from waste water treatment and Hydrotreated C6 (producers of these two streams indicated that the streams were not isolated in the year that the use data were collected), and Pyrolysis C6s (specific use data were not available from the producers of this stream).

FIGURE 2
USE OF THE HIGH BENZENE NAPHTHA
CATEGORY STREAMS (2001 DATA)²



Route of Potential Exposure: The category streams are liquids at ambient conditions, with volatility similar to gasoline. Inhalation is a likely route of potential exposure due to the volatility of the streams. There is also a potential for dermal exposure as a result of accidental contact. The streams or components in the streams are slightly soluble in water and therefore groundwater contamination is possible in the event of spills or leaks from processing,

² The percentage uses of the category streams are based on data received from 14 of the original 16 category sponsors. Although similar information was not available from the other sponsor at the time this report was written, the uses shown in Figure 2 are expected to be representative of the industry. Uses of 3 of the category streams are not included in Figure 2, because the streams were either not isolated during the reporting year, or the specific use information was not available from the sponsors of the streams at the time this report was written.

transportation or storage equipment. All of these streams contain significant concentrations of benzene.

Sources of Potential Exposure: Exposure to the category streams for workers in the Olefins Industry process units where the category streams are isolated or used is expected to be low because that equipment and those processes are closed systems. Emissions from storage and loading equipment are typically controlled by using floating roof storage tanks or by routing vents from fixed roof storage tanks and loading equipment to control or recovery systems, or back to the process. For the industrial workers at these facilities, the most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from valve packing and from pump seals. There is also potential for exposure during operations such as sampling, loading of bulk transportation vessels (tank cars and barges), from emissions at floating roof storage tanks, during infrequent opening of equipment for maintenance, or from emissions from control devices, such as flares.

The above-described sources of emissions of the category streams may present a potential for exposure to the public and to the environment adjacent to the industrial facilities that use or produce the category streams.

All of the category streams contain significant concentrations of benzene. "Emissions of benzene to the atmosphere result from gasoline vapors, auto exhaust, and chemical production and user facilities."³ "Occupational exposure to benzene may occur through inhalation and dermal contact with this compound at workplaces where benzene is produced or used. The general population may be exposed to benzene via inhalation of ambient air, ingestion of drinking water, and dermal contact with gasoline products containing benzene..⁴ EPA's Total Exposure Assessment Monitoring (TEAM) studies carried out between 1980 and 1990 indicate that for chemicals such as benzene, "the most important sources of pollution are small and close to the person, and that exposures are not clearly correlated with emissions. For example, the TEAM study findings indicated that, although nearly 85% of atmospheric benzene in outdoor air is produced by cars burning petroleum products and the remaining 15% is produced by industry, about half of the total national exposure to benzene comes from cigarette smoke."³

Controls that Limit Exposure: The OSHA Benzene Standard applies to the streams in the High Benzene Naphthas category and thus limits occupational exposure to the streams. The Standard requires controls and work practices that limit benzene occupational exposure to less than 1 ppm, 8-hour TWA and a short-term level of 5 ppm (15 minute)⁵. In addition, the OSHA Standard establishes an action level of 0.5 ppm (8-hour TWA). Since benzene is a primary component of all the category streams, these limits on benzene occupational exposure effectively limits occupational exposure to the category streams.

³ <http://atsdr1.atsdr.cdc.gov/toxprofiles/tp3-c5.pdf> (ATSDR Toxicological Profile for Benzene), September 1997 updates

⁴ <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB> (HSDB references 1986 to 1997 sources for at least a portion of this information.) (HSDB references 1986 to 1997 sources for at least a portion of this information.)

⁵ OSHA Standard for Benzene: 29 CFR 1910.1028.

http://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=10042

In addition OSHA and ACGIH have established guidelines for some components in the category streams. For example, the OSHA PEL for Toluene (a component in most of the category streams) is 200 ppm; and the ACGIH TLV is 50 ppm. Eleven of the original sixteen sponsors of the category streams reported that they have programs that assess exposure to the category streams, including specific measurements for benzene. Industrial hygiene programs for a specific production site are typically unique to the site and address the specific chemical exposure issues. Some of the components typically present in the category streams and that have OSHA PELs or ACGIH TLVs are shown in Table 5.

Table 5. Components Typically Present in Some Streams in the High Benzene Naphthas Category & That Have OSHA PELs or ACGIH TLVs

Component	OSHA PEL	ACGIH TLV	Component	OSHA PEL	ACGIH TLV	Component	OSHA PEL	ACGIH TLV
Benzene ^a	1	0.5	Ethylbenzene	100	100	Styrene	100	20
Biphenyl	0.2	0.2	Heptane	500	400	Toluene	200	50
Cumene	50	50	Indene	-	10	Vinyltoluene	100	50
CPD ^b	75	75	Naphthalene	10	10	Mixed Xylenes (o-, m-, p - Isomers)	100	100
Cyclopentane	--	600	Octane isomer	500	300			
DCPD ^c	-	5	Pentane Isomers	1000	600			

^a Benzene OSHA Action Limit is 0.5 ppm

^b CPD: Cyclopentadiene

^c DCPD: Dicyclopentadiene

Among other reasons, the release of the category streams from process, storage and transportation equipment at industrial facilities is avoided because the streams are flammable liquids, similar in flammability and volatility characteristics to gasoline.

The category streams are mixtures of volatile organic compounds (VOC) and are therefore subject to multiple US EPA and state environmental regulations that limit VOC emissions. Limits on emissions of the components of the category streams effectively limits exposures to the category streams. The US EPA new source performance standards (NSPS) of 40 CFR Part 60 may be applicable and limit emissions of VOC at new or modified Olefins process units where the streams in the category are produced and used. Subpart VV of NSPS limits emission from equipment leaks, subpart NNN limits emissions from distillation operations, subpart RRR limits emissions from reactor systems and subpart Kb limits emissions from VOC storage tanks. The category streams contain benzene and are typically subject the National Emissions Standard for Hazardous Air Pollutants (NESHAPs) of 40 CFR Part 61. NESHAP subpart J and V limit emissions of benzene from equipment leaks, subpart FF limits emissions from benzene wastes, subpart Y limits emissions from benzene storage tanks, and subpart BB limits emissions from benzene transfer operations. In addition, facilities that produce or use these streams and that are major sources may be subject to the National Emission Standards for Hazardous Air Pollutants for Source Categories: Generic Maximum Achievable Control Technology Standards, which includes ethylene manufacturing processes and may be subject to the Hazardous Organic

NESHAP (HON), 40 CFR Part 63, subpart F, G and H. Facilities that produce and use the category streams are also typically subject to state operating permits and state regulations that further limit VOC emissions. These emissions control requirements effectively limit exposure potentials for the category streams for both workers at the facilities and the neighboring public and environment.

Ambient Air Concentration Data: Ambient air concentration data for the complex category streams are not available. However, all of the category streams contain significant concentrations of benzene.

“Atmospheric benzene concentrations were studied throughout the USA between 1977-1980 in which out of 487 samples taken, benzene was found at an average concentration of 3.0 ppb. The concentration of benzene near USA chemical factories where benzene is used ranged from 0.6-34 ppb, near service stations 0.0003-3.2 ppm, and in cigarette smoke 57-64 ppm.”⁴ Ambient air concentrations (1994 through 1997) for benzene at selected industrial sites in Texas are available from the Texas Community Air Toxics Monitoring Network⁶. Calculated values from that data indicate an average annual mean value of 0.96 ppb, with a range of from 0.22 to 7.0 ppb, and an average of the 24-hour annual high values of 5.03 ppb, with a range of from 0.34 to 63.63 ppb.

Estimates of Potentially Exposed Workers: NIOSH (NOES Survey 1981-1983) has statistically estimated that 272,275 workers (143,066 of these are female) are potentially exposed to benzene in the US⁴. A number of limitations to this survey have been identified over the years, and the estimates of the number of workers potentially exposed to various substances are generally thought to be high.

Category emissions: Emissions quantities of the mixed streams are not available. Benzene is a component found at significant concentrations in all of the category streams. Emissions of benzene in these category streams are included in the industrial emissions of benzene that are reported to the EPA and made available to the public in the Toxics Release Inventory (TRI) ⁷. This inventory was established under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) and expanded by the Pollution Prevention Act of 1990.

The TRI data indicate that emissions of benzene have significantly decreased since 1988 (Figure 3). The TRI data from 2002 indicate that emissions and disposal quantities of benzene reported in the TRI for the chemical sector (SIC 28) have declined by 81% since 1988, and the number is down 79.7% for all US industries. However the relevance of individual component emissions values with regard to the category streams is uncertain, because the category streams likely account for a minor portion of the total emissions for specific components.

⁶ <http://www.tnrcc.state.tx.us/air/monops/cat97/cat97.html>

⁷ EPA website for TRI: <http://www.epa.gov/tri/>

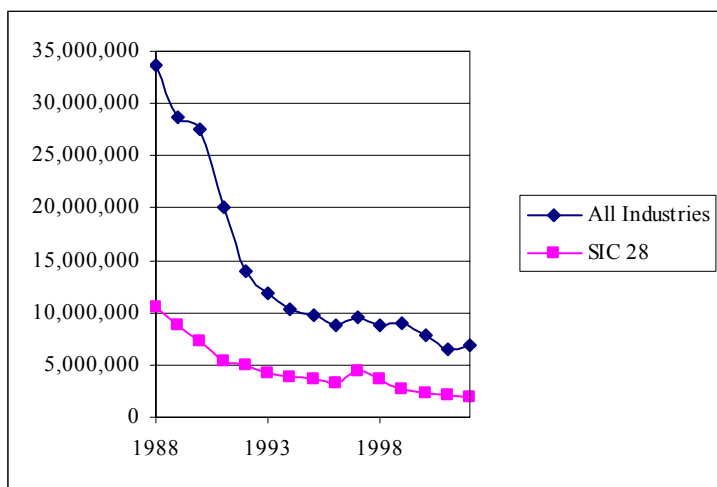


Figure 3
TRI Benzene Total
Disposal & Emissions
(lbs/year) for All
Industries and for the
Chemical Sector (SIC
28) 1988 - 2002

2.1 Summary of Exposure Assessment

The HPV High Benzene Naphthas Category includes the ten isolated product streams from the Olefins Industry that contain significant concentrations of benzene. Nineteen CAS numbers are used to represent these streams. The category streams are complex mixtures of variable composition. Benzene is separated from the category streams, or from other intermediate streams derived from the category streams, in downstream process units.

There are no expected consumer applications for these materials.

The category streams are typically used at the same location where they are produced or transported to other industrial facilities in bulk by pipeline, barge, tank car or tank truck.

Inhalation is a likely route of potential exposure due to the volatility of the hydrocarbon components that make up the streams. Other possible exposure routes include dermal (from spills) and oral (from contaminated ground water).

Occupational exposure is limited because production and use of these streams is in closed systems, and the requirements of the OSHA Benzene Standard limits occupational exposure to benzene. Benzene is a common, primary component of all these streams. OSHA and ACGIH exposure limits also exist for several of the other components of the category streams.

Environmental exposure is limited since emissions from production and use are limited and controlled by a number of volatile organic compound and hazardous air pollutant environmental regulations at both the federal and state level. The category streams are produced, transported and used in closed systems. The subsequent processing of the process streams in this HPV Category ultimately result in the production of other products (e.g. benzene and other non-benzene containing products) and the consumption of the original category streams.

3. ENVIRONMENTAL FATE

3.1 Photodegradation

3.1.1 Direct Photodegradation:

The absorption of light in the ultraviolet (UV) visible range (110-750nm) can induce electronic excitation of an organic molecule. The stratospheric ozone layer allows only light in wavelengths in the 290-750nm range to reach earth's surface with the potential to result in photochemical transformation in the environment. To estimate photochemical degradation, it is assumed that degradation will occur in proportion to the amount of light wavelengths greater than 290nm absorbed by the molecule. Saturated hydrocarbons do not absorb appreciable light energy above 200nm. Olefins with one double bond or two conjugated double bonds, which constitute the majority of chemicals in the High Benzene Naphthas category, do not absorb appreciable light energy above 290nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjunction with an aromatic ring [Harris et al., 1982]. Examples of absorbance maxima (λ_{\max}) and associated molar absorptivities (ϵ) for representative hydrocarbons are shown below.

Table 6. Characteristic Absorbance Maxima (λ_{\max}) and Associated Molar Absorptivities (ϵ) for Representative Hydrocarbons of the High Benzene Naphthas Category

Hydrocarbon	λ below 290 nm		λ above 290 nm	
	λ_{\max}	ϵ	λ_{\max}	ϵ
Ethylene	193	10,000	--	--
Benzene	255	215	--	--
Styrene	244 282	12,000 450	--	--
Naphthalene	221 270	100,000 5,000	311	250

Only naphthalene demonstrated some photochemical degradation at wavelengths above 290nm.

Products in the High Benzene Naphthas category do not contain component molecules that will undergo direct photolysis, with the exception of naphthalene. This process will not contribute a measurable degradative removal of chemical components in this category from the environment.

3.1.2 Indirect Photodegradation (Atmospheric Oxidation):

Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation but an indirect degradation process. Hydrocarbons such as those in the High Benzene Naphthas Category have the potential to volatilize to air where they can react with hydroxyl radicals (OH \cdot). The rate at which an organic compound reacts with OH \cdot radicals is a direct measure of its atmospheric persistence. The AOPWIN version 1.89 computer program (subroutine of EPIWIN 3.04) was used here to estimate the rate constants for OH \cdot radical reactions of representative organic constituents of the products in the High Benzene Naphthas

category, which are then used to calculate atmospheric half-lives for these constituents as shown below:

Table 7. Hydroxy Radical Photodegradation Half-lives of Representative Hydrocarbons of the High Benzene Naphthas Category

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm ³ /molecule-sec)
Isopentane	1.2	105.1 E ⁻¹²
n-pentane	31.7	4.0 E ⁻¹²
1,3-cyclopentadiene	0.9	142.6 E ⁻¹²
Isohexane	22.4	5.7 E ⁻¹²
n-hexane	23.5	5.5 E ⁻¹²
Methylcyclopentane	22.7	5.7 E ⁻¹²
Benzene	65.8	1.9 E ⁻¹²
Toluene	24.6	5.2 E ⁻¹²
m-xylene	9.5	13.6 E ⁻¹²
Styrene	4.6	28.1 E ⁻¹²
Dicyclopentadiene	1.1	119.2 E ⁻¹²
Naphthalene	5.9	21.6 E ⁻¹²

* Atmospheric half-life values are based on a 12-hr day.

Based on these calculated values, for representative stream constituents, products in the High Benzene Naphthas category can have an atmospheric half-life range of 0.9 –65.8 hours, indicating that atmospheric oxidation can be a significant route of degradation for products in this category.

3.2 Stability in Water

Hydrolysis is unlikely for product streams in the High Benzene Naphthas category. Hydrolysis is a nucleophilic substitution reaction in which a water molecule or hydroxide ion reacts with an organic molecule to form a new carbon-oxygen bond. Carbon to carbon double bonds are too stable to be cleaved by nucleophilic substitution and the carbon atom lacks sufficient electronegativity to be a good “leaving group”. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters and sulfonic acid esters. The chemical components of the High Benzene Naphthas are hydrocarbons that are not included in these groups and have very low potential to hydrolyze. This degradative process will not contribute to removal of these hydrocarbons in the environment.

3.3 Distribution in the Environment

Substances in the High Benzene Naphthas category are calculated to partition primarily into air with negligible percentages partitioning in water, soil and sediment. Relatively high vapor pressure and low water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.

The EQC level 1 fugacity model (Mackay et al., 1996) recommended by U.S. EPA (1999b) was used to determine partitioning of representative chemical constituents into different environmental compartments under steady state conditions, in order to estimate the partitioning behavior for the category substances. Mackay level 1 distribution values, calculated and measured, for 12 representative constituents of products in this category are presented below:

Table 8. Environmental Distribution as Calculated by EQC Level I Fugacity Model for Representative Hydrocarbons of the High Benzene Naphthas Category

Chemical	Percent Distribution: Calculated ^a [Measured] ^b			
	Air	Water	Soil	Sediment
Isoprene	99.97 [99.96]	0.02 [0.03]	0.01 [0.01]	-
n-pentane	99.97 [99.99]	0.02 [0.01]	0.01 [-]	-
1,3-cyclo-pentadiene	99.93 [99.93]	0.06 [0.06]	0.01 [0.01]	-
Isohexane	99.96 [99.97]	0.02 [0.01]	0.02 [0.02]	-
n-hexane	99.95 [99.96]	0.02 [-]	0.02 [0.04]	-
Methylcyclo-pentane	99.94 [99.95]	0.03 [0.02]	0.03 [0.03]	-
Benzene	98.46 [98.89]	1.42 [1.00]	0.12 [0.11]	-
Toluene	98.17 [98.80]	1.40 [0.81]	0.43 [0.39]	-
m-Xylene	97.19 [97.91]	1.33 [0.86]	1.45 [1.20]	0.03 [0.03]
Styrene	95.55 [96.65]	2.61 [1.85]	1.80 [1.46]	0.04 [0.04]
Dicyclo-pentadiene	98.00 [98.55]	0.87 [0.63]	1.11 [0.80]	0.02 [0.02]
Naphthalene	24.47 [42.27]	32.28 [20.56]	42.28 [36.33]	0.94 [0.81]

a- Values determined using calculated input data from EPIWIN program

b- Values determined using input data from the EPIWIN program experimental database.

With the exception of naphthalene, the representative components partition into air at >95%; water 0.01 – 2.61%; soil 0.01 – 1.8% and sediment <1.0%.

3.4 Biodegradation

There are sufficient data to characterize the potential biodegradability of products in this category. Data for constituent chemicals of products in this category (as well as for complex products not in this category that contain chemicals found in products from this category) suggest that high benzene naphtha products have the potential to biodegrade to a great extent (Appendix 5, Table A5-1). The carbon number of products in this category ranges primarily

between C5 to C11. Results for several chemicals, including benzene, with carbon numbers in this range that are contained by these products have been shown to biodegrade from 63 to 100% after 14 or 28 days, while results for several comparable, complex streams containing several components range from 21 to 96% after 28 days. As seen by the data in Table A5-1, there is a relatively large biodegradation database for single chemicals and complex streams that can be used to characterize this endpoint for high benzene naphtha products. Because products in this category are compositionally more comparable to the products identified in Table A5-1 as gasoline streams (although gasoline streams contain less benzene), these data best describe the potential biodegradability of the high benzene naphtha streams. Gasoline stream compositions are provided in Table A5-2.

The data from the majority of tests in Table A5-1 were developed using a manometric respirometry test procedure. This procedure uses continuously stirred, closed systems, which is recommended when assessing the potential biodegradability of chemically complex, poorly water soluble, and volatile materials like those in this category. Stirring is recommended when evaluating products containing several chemicals, some of which may have limited water solubility. The manometric respirometry test of benzene [Robust summary in Attachment 1b] indicates that benzene is readily biodegradable with a half-life of less than 2 weeks. By day 28, 63% degradation had occurred; 10% biodegradation was achieved in less than 5 days with 50% biodegradation by approximately day 5.

4. HUMAN HEALTH HAZARDS

4.1 Effects on Human Health

The 10 streams in the High Benzene Naphthas Category are commercial hydrocarbon products or isolated intermediates derived from Ethylene manufacturing and contain significant levels of benzene, averaging 55% [range of 10-80%]. The toxicity and epidemiology databases for benzene and other components of this category as well as mixtures containing the components, are extensive. Health effects data on components present in the streams is summarized in Appendix 3, Table A3-1.

Pyrolysis gasoline is the major stream in this category and data are available for 3 streams: Data for Pyrolysis gasoline [Dripolene], a C5-C10 distillate fraction of a pyrolysis gasoline [Rerun Tower Overheads] and the hydrotreated C6-C8 fraction [Hydrogenated Pyrolysis Gasoline] are summarized below and presented in Robust Summaries in Attachment 1c.

Benzene is the likely key driver for health effects, primarily in genotoxicity and hematotoxicity for HPV endpoints. All components present in the streams at concentrations greater than 5% have been tested in at least one toxicity study. Those components having only limited data lack structural alerts for mammalian toxicity and data exist for their structural analogs. The C5 and C6 alkanes and alkenes present in the streams are not expected to significantly contribute to the toxicity profile as these substances are present in the streams at low concentrations and, with the exception of hexane, generally have a low level of toxicity. The toxic effects of hexane (present at $\leq 15\%$) are unlikely to be observed due to the presence of and interaction with other components.

Chemical Component Interactions

When tested as pure substances, some of the components in the High Benzene Naphthas streams other than benzene have caused genetic damage and adverse target organ effects in repeated-dose animal studies. However, since the biologically active components of the High Benzene Naphtha streams are metabolized through a common P450 metabolic pathway, it is anticipated that multiple components will compete for the same active enzyme sites. Component toxicities, which are dependent on the formation of biologically active metabolites, may be reduced as less metabolite(s) will be produced through competition for these sites. Direct support for reduction or elimination of toxicities of individual components is provided by results of an existing mouse bone marrow micronucleus test with one of the High Benzene Naphtha streams, Hydrotreated C6-8 Fraction described in the summary of *in vivo* mutagenicity data below. This stream, containing approximately 55% benzene, was negative in a mouse bone marrow micronucleus test when administered by oral gavage at 2000 mg/kg to male and female CD-1 mice (see robust summary). Several studies have shown that benzene administered orally to CD-1 mice induces high frequencies of micronuclei in bone marrow erythrocytes at doses as low as 110 mg/kg (Ciranni et al., 1988; Suzuki et al., 1989; Hite et al., 1980; Gad-El Karim et al., 1986; Meyne and Legator, 1980). The presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene. Other similar interactions between components of the category have also been reported, as noted below.

Medinsky et al. (1994) and Bond et al. (1998) reviewed the metabolism of benzene and the effects of interactions with other organic chemicals on benzene toxicity and metabolism. Reports of interactions between other components of the High Benzene Naphthas Category have also been noted in the literature. Examples of these interactions and the effect on the formation of benzene metabolites and resultant hematotoxicity or genotoxicity are shown below:

- When benzene (440 mg/kg) and toluene (430, 860, or 1720 mg/kg) were coadministered orally to mice, the clastogenic effect of benzene was reduced (Gad-El-Karim et al., 1984, 1986).
- Coadministration of toluene (1720 mg/kg), i.p., with benzene (440 and 880 mg/kg) to mice resulted in a reduction in the quantity of benzene metabolites measured in the urine (Andrews et al., 1977). Coexposure to toluene also protected against benzene-induced depression in ⁵⁹Fe utilization by red blood cells, which is used as a measure of hematotoxicity.
- Coexposure to 2000 ppm fully vaporized or light gasoline components reduced the incidence of genetic damage (micronuclei in bone marrow) resulting from a single 6-hr exposure to 40 ppm benzene (Bond et al., 1998). The major components of the fully vaporized gasoline and light gasoline mixtures, respectively, were n-butane (6.1%, 23.9%), n-pentane (3.7%, 8.4%), isopentane (12.3%, 33.5%), n-heptane (1.2%, 0.3%), toluene (8.2%, 1.1%), ethylbenzene (2.3%, 0.1%), and xylenes (8.4%, 0.2%). In these experiments, the fully vaporized gasoline mixture, which contained a higher fraction of aromatic hydrocarbons, was a more effective inhibitor of benzene metabolism than was the light fraction, which was composed primarily of aliphatic hydrocarbons.
- Results of studies with styrene-butadiene mixtures showed a decrease in the rate of metabolism of each chemical but an increase in the concentration of the circulating epoxide

metabolites (Bond et al., 1998). The frequency of micronuclei seen in mice exposed by inhalation to butadiene was not altered by simultaneous exposure to styrene.

- Synergistic losses of auditory sensitivity occurred following combined exposure of rats to vapors of toluene plus n-hexane and xylene plus n-hexane (Nylen, 1996). These combined exposures, however, produced antagonistic effects in nerve conduction or action potential amplitudes in the auditory pathway, visual pathway, and peripheral nerve.
- Exposure of male rats to 1000 ppm n-hexane for 61 days caused testicular atrophy and loss of germ cell line (Nylen, 1989). Simultaneous administration of 1000 ppm toluene or xylene did not cause germ cell line alterations or testicular atrophy.
- Neurological effects have been observed in many intermediate-duration inhalation experiments in rats exposed to n-hexane (ATSDR, 1999). No neurotoxic effects were observed in a 2-year chronic study in rats and mice with commercial hexane containing 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane (Daughtrey et al., 1999). In a separate 13-week inhalation study of commercial hexane, a detailed neurobehavioral/neuropathological evaluation revealed no n-hexane-induced neuropathy (Soiefer et al., 1991).

4.1.1 Acute Toxicity

Studies in Animals

Table 9. Summary of Acute Toxicity Data for Representative Streams and Components in the High Benzene Naphthas Category

Route	Dripolene	Hydrotreated C6-8 stream (Hydrogenated Pyrolysis Gasoline)	C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads)	Benzene ^a	Toluene ^a
Oral LD50	>2.0g/kg	5.17g/kg	>2.0g/kg	0.81-1.0g/kg	5.5g/kg
Dermal LD50	> 2.0g/kg	---	>2.0g/kg	---	12.4g/kg
Inhalation LC50 [4hr exposure]	---	>12,408ppm	---	13,700ppm	8000-8800ppm

a- data from Table A3-1

Conclusion

High benzene naphtha streams demonstrate minimal toxicity by oral, dermal or inhalation routes of exposure. With the exception of dicyclopentadiene (see Table A3-1) the components of these streams demonstrate overall low levels of acute toxicity as well.

4.1.2 Repeated Dose Toxicity

Studies in Animals

Two streams were tested in repeated-dose studies. A 5-day rat inhalation study was conducted with a Hydrotreated C6-8 stream (Hydrogenated Pyrolysis Gasoline), and a 21-day rabbit dermal

irritation study, which included evaluations for systemic effects, was conducted with a C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads).

Inhalation

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis gasoline) was evaluated for toxicity in a 5 day inhalation study using F344 rats. Animals (5/sex/group) were exposed at concentrations of 0, 4869 and 9137ppm daily for 5 days and sacrificed on day 8 after a 2-day post-exposure observation period. Three rats (1M, 2F) from the high dose group died on day 1-2 of exposure. Rats were lethargic and showed labored respiration on days 1-5 of treatment but all but one high dose rat recovered fully by day 8. Group mean body weights were significantly decreased in a dose-related manner but no test material-related effects were reported at gross necropsy. NOAEL <4869ppm

Dermal

C5-C10 fraction of Pyrolysis Gasoline (Rerun Tower Overheads) was evaluated for skin irritation and systemic toxicity in a 21-day dermal study using New Zealand White rabbits. Test material [undiluted] was applied to the shaved abraded back of 4M and 4F rabbits per group at concentrations of 0, 0.1, 0.5, and 1.0ml once a day for 21 consecutive days. Exposed sites were unoccluded and each rabbit wore a Plexiglas collar to retard ingestion of test material. Skin irritation and erythema were observed in a dose-related manner. No significant effects were seen on body or organ weight, feed consumption, hematology or serum chemistries. No abnormal microscopic changes were observed in any organ system with the exception of damage to dermal layers consistent with gross observations of irritation. NOAEL (irritation) <0.10ml/kg; NOAEL (systemic) =1.0ml/kg.

Oral

No studies are available for these streams.

Conclusion

Inhalation exposure to Hydrotreated C6-C8 stream produced lethargy and labored respiration, effects from which most rats recovered after 2 days without exposure. Dermal exposure to the C5-C10 fraction of Pyrolysis gasoline induced skin irritation in rabbits but no other systemic toxicity.

The effects reported for these representatives of the High Benzene Naphthas category are similar to those observed for gasoline blending streams (API HPV test plan, 2003) in which dermal treatment induced primarily skin irritation and concomitant systemic effects and inhalation exposure-induced effects on lung, liver, kidney and blood occurred at high doses and were no longer observed after 4 weeks of recovery in most studies.

Repeated oral or inhalation exposures to many of the components of the streams in the category have been shown to cause adverse health effects in a variety of organs. Of the components summarized in Table A3-1, benzene demonstrated toxicity primarily in the hematopoietic system, toluene affected the central nervous system and induced loss of auditory sensitivity, and light hydrocarbon nephropathy was seen with exposure to hexane isomers, a 50/50 blend of n-butane and n-pentane, or with dicyclopentadiene. However, existing data also show that

antagonistic and synergistic interactions occur between some components comprising the streams, as noted above in the Chemical Component Interaction section of the Introduction to Section 4.1, which alter the effects of individual hydrocarbons. The target organs affected by exposure to the mixtures, and the severity of the effects, depend upon the relative concentrations of the components within each stream and the nature of the interactions between components.

Many of the C5 components of the High Benzene Naphthas Category are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) being tested for repeated-dose toxicity by the Panel, as part of the HPV Program. Based on structural similarity, pentenes are likely to have a toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel addresses hexenes as part of the HPV Program. Also, the International Hydrocarbon Solvents Consortium covers the C5 aliphatic components in its C5 Aliphatics Category. Pentane is being addressed in the American Petroleum Institute's Petroleum Gases Test Plan. Other components are shared with the Panel's Resin Oils and Cyclodiene Dimer Concentrates Category streams. Several components are sponsored in the OECD SIDS or ICCA programs (see Table A3-1). Results of these studies will supplement the current assessment as data become available.

The most conservative assessment for repeated-dose human health hazards would be based on toxicity results for individual components (e.g. benzene). However data from testing of similar streams suggest the actual toxicity may be somewhat less in these blended streams due to lower concentrations, component interaction and competitive inhibition of biologically active hydrocarbon constituents.

4.1.3 Mutagenicity

In vivo Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline) was evaluated for cytogenetic damage in the mammalian bone marrow erythrocyte micronucleus assay using male and female Swiss mice. Mice were given oral doses of 0, 0.5, 1.0, or 2.0g/kg/day for 2 days or 1 dose of 2.0g/kg for one day. Treatment did not increase the frequency of micronucleated polychromatic erythrocytes in mouse bone marrow.

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) was tested in *Drosophila melanogaster* for gene (point) mutations and cytogenetic damage (chromosome loss or aberrations). The stream did not induce gene mutation or chromosome damage in this fruit fly system

In vitro Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline) did not induce mutagenic events in 4 strains of *Salmonella typhimurium* or one strain of *Escherichia coli* with or without metabolic activation from rat liver S9. This stream also did not induce unscheduled DNA synthesis in primary rat hepatocytes.

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) did not induce mutagenic events in 5 strains of *Salmonella typhimurium* with or without metabolic activation from rat liver S9.

However, this stream did cause weak differential killing in DNA repair-deficient strains of *E. coli* and *S. typhimurium*. In mammalian cells, a weak positive response in mouse lymphoma cells without metabolic activation was induced but no increase in revertant colonies with metabolic activation was seen.

Conclusion

Chromosome aberrations: The representative streams tested did not induce cytogenetic damage in animals. Indeed, Hydrotreated C6-C8 demonstrated how interaction and competition for metabolic sites can block toxicity of individual components. Although containing 55% benzene, the presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene.

Although benzene has caused chromosome aberrations *in vivo* and *in vitro*, toluene, the other most prevalent component in this category, is not clastogenic. Of the remaining identified category components present at concentrations greater than 5%, only vinyl acetate, 1,3-butadiene, isoprene, hexane, and naphthalene have been reported to cause chromosome aberrations (see Table A3-1). As discussed above and in the introduction to Sect.4.1, coadministration of benzene with other hydrocarbons that are substrates for the cytochrome P450 enzymes can reduce clastogenicity. Additional information that may be useful will become available from mouse micronucleus testing conducted with streams distilled from Pyrolysis Gasoline that are members of the Panel's C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories.

Gene mutation: Neither stream induced gene mutation in bacterial systems. Although the C5-C10 fraction of Pyrolysis gasoline did cause a direct weak positive response in mammalian cells, inclusion of metabolic activation in the test system did not cause mutation, indicating that detoxification of the test material had occurred. The suggestion of genetic toxicity posed by this weak mutational activity and weak differential killing in repair-deficient strains of bacteria was not confirmed *in vivo*. No gene mutation or clastogenic events were observed in the sensitive *Drosophila* test system. Most of the stream components (Table A3-1) with the exception of 1,3-butadiene did not induce mutation in bacteria and are not considered gene mutagens.

Thus, based on composition and available data for representative streams, components and mixtures of components, it is unlikely that most streams in the High Benzene Naphthas category are gene mutagens or are significantly clastogenic.

4.1.4 Carcinogenicity [Non-HPV SIDS Endpoint]

In vivo Studies

No studies are available on high benzene naphtha streams. Of significant components, benzene is a demonstrated leukemogen in humans (acute myelogenous leukemia) and induces solid tumors in laboratory animals. However, toluene, also a major constituent of the High Benzene Naphthas Category streams, and a competitor with benzene for metabolic sites did not induce tumors at concentrations as high as 1200ppm in a 2-year inhalation study in rats and mice (NTP, 1990). In a 2-year inhalation study of wholly vaporized gasoline (MacFarland et al., 1984), the principal

tumorigenic effect occurred in kidneys of male rats and was later demonstrated to be a species and sex specific event unrelated to health hazards for man (US EPA, 1991).

In vitro Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline) caused cell transformation in BALB-c/3T3 cells at a high concentration of 5000ug/ml, a level that was too toxic for cells to recover and form colonies.

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) did not induce cell transformation in two test systems; the mouse embryo C3H 10T1/2 cell line or the BALB-c/3T3 cell line

Conclusions

Cell transformation assays on representative streams demonstrated minimal if any carcinogenic potential. Transformation induced by the Hydrotreated C6-C8 stream occurred at a high dose from which cells are unlikely to survive and produce potentially tumorigenic colonies, and the C5-C10 fraction did not induce cell transformation.

Although no carcinogenesis studies were available on high benzene naphtha streams, extrapolation from 2-year cancer bioassays on gasoline and toluene, and the apparent competitive detoxifying effects of toluene when co-administered with benzene seen in other studies, suggest that carcinogenesis is unlikely to be a significant endpoint of toxicity for this naphtha category.

4.1.5 Toxicity for Reproduction

Effects on Fertility

No reproductive toxicity studies are available on high benzene naphtha streams. However, data are available on many components in reproductive studies and/or pathological evaluations of reproductive organs in systemic toxicity studies (see Table A3-1). In its review of benzene, ATSDR (1997) concluded that, although there are some data indicating adverse gonadal effects (e.g., atrophy/degeneration, decrease in spermatozoa, moderate increases in abnormal sperm forms), data on reproductive outcomes are either inconclusive or conflicting. However, most studies indicate no effects on reproductive indices, even at high doses. Reproductive organ effects were seen after inhalation exposure to isoprene and hexane in subchronic toxicity studies but such effects may not affect reproductive capabilities in practice. However, for hydrocarbons tested in multi-generation reproductive studies – toluene, cyclohexane, pentane, commercial hexane (isomers), mixed xylenes, and styrene, no effects on fertility or other reproductive parameters were reported. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation two-generation reproductive toxicity study. Dicyclopentadiene demonstrated reproductive effects in a 3-generation reproductive study only at maternally toxic doses.

For other chemical components present in High Benzene Naphtha streams, data generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause reproductive effects. Some of these materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that being tested for

reproductive toxicity by the Panel, as part of the HPV Program. Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes, which will be addressed by the American Chemistry Council's Higher Olefins Panel as part of the HPV Program. Pentenes are also covered by the American Chemistry Council's Hydrocarbon Solvents Panel (C5 Aliphatics Test Plan). Additional reproductive toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline. 1,3-Butadiene is being tested for reproductive effects in the OECD SIDS program.

Developmental Toxicity

C5-C10 fraction of Pyrolysis gasoline (Rerun tower overheads) was tested for developmental toxicity in New Zealand White rabbits at oral gavage doses of 0, 10, 25 and 50mg/kg/day from days 6-28 of gestation. One rabbit given 50mg/kg/day aborted on day 19 but all other animals completed gestation. Maternal body weights were comparable to controls throughout gestation. There were no biologically or statistically significant differences in pregnancy ratios, number of corpora lutea, total implantations, resorptions, postimplantation loss, viable fetuses, litter size, fetal sex index, or mean fetal body weights. No statistically significant differences in number of litters with malformations were reported. C5-C10 fraction did not produce a teratogenic response in New Zealand White rabbits. Maternal NOAEL = 25mg/kg/day. Developmental NOAEL = 50mg/kg/day.

In addition to this study on a representative stream of the High Benzene Naphthas Category, developmental toxicity data exist for most components present in this category at concentrations greater than 5% (see Table A3-1). In these studies, no convincing evidence was seen for teratogenicity in the absence of maternal toxicity. Fetotoxicity has been reported for some components, but mostly in the presence of maternal toxicity (see Table A3-1). Only five components (pentenes, cyclopentene, 3-methylpentane, methylcyclopentane, 1,3-cyclopentadiene) lack developmental toxicity tests. However, these components do not have structural alerts for developmental toxicity, and data being generated by other test plans within the HPV Program will provide additional information about the potential of these substances to cause developmental effects. Three of the five chemicals are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that are being tested for developmental toxicity by the Panel, as part of the HPV Program. Pentenes are addressed by the International Hydrocarbon Solvents Consortium (C5 Aliphatics Test Plan). Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel address hexenes as part of the HPV Program. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation developmental toxicity study. Additional developmental toxicity information will become available from testing conducted by the Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category with streams distilled from Pyrolysis Gasoline.

Conclusion

On the basis of available data, High Benzene Naphtha streams seem unlikely to cause significant reproductive or developmental toxicity. Reproductive studies on components present in these streams overall gave negative results. The C5-C10 fraction of Pyrolysis gasoline, a

representative high benzene naphtha stream did not induce developmental effects in rabbits and stream components that induced developmental toxicity did so primarily at doses that were also toxic to the dam. Additional data from the ongoing programs cited above will provide further supplementary data.

4.2 Assessment Summary for Human Health

Existing data are sufficient to characterize human health hazards of substances included in the High Benzene Naphthas Category and thus, satisfy HPV testing requirements. From data on representative streams, and read-across from chemical components and analogous streams, it can be concluded that High Benzene Naphthas are not acutely toxic by the oral, dermal or inhalation routes of exposure.

Although these streams contain substantial concentrations of benzene, they are unlikely to induce genetic damage *in vivo*, as demonstrated by the absence of clastogenicity induced by oral exposure to the Hydrotreated C6-C8 stream and the absence of gene mutation or chromosome damage in *Drosophila* exposed to the C5-C10 fraction of Pyrolysis gasoline. Mixtures of benzene with other hydrocarbons such as toluene and gasoline have resulted in inhibition of benzene chromosome damage potential. In addition, most stream components did not induce mutation in bacteria.

Repeated dose toxicity studies of two representative streams of the High Benzene Naphthas category showed results similar to those observed for analogous gasoline blending streams. Dermal exposure produced primarily skin irritation and concomitant systemic effects. Lethargy and labored respiration induced by limited duration inhalation exposure at high doses were resolved after treatment was terminated. The high content of benzene in these streams dictates that, from a conservative perspective, the systemic hazards from components be considered hazards for the streams until sufficient data becomes available to show the specific combination of components does not present the hazard. However, it is probable that any systemic toxicity demonstrated in laboratory animals would occur at doses well in excess of established workplace standards.

Based on available data, no significant reproductive or developmental toxicity is likely to result from exposure to streams in the High Benzene Naphthas category. Reproductive studies on components present in these streams overall gave negative results. The C5-C10 fraction of Pyrolysis gasoline did not induce developmental toxicity in rabbits and stream components that were biologically active caused effects primarily at high doses that were maternally toxic. Again, established workplace standards for components are sufficient to protect against human health hazards from exposure to member streams of the High Benzene Naphthas category.

The compositional similarities of these streams and consistency of data from mammalian studies using representative streams and components of these streams, along with published toxicity data from other naphtha streams in this boiling range, justifies the designation of the High Benzene Naphthas as a category for HPV.

5. HAZARDS TO THE ENVIRONMENT

5.1 Aquatic Effects

Acute Toxicity

The aquatic toxicity endpoints for the HPV Chemical Program include:

- Acute Toxicity to a Freshwater Fish
- Acute Toxicity to a Freshwater Invertebrate
- Toxicity to a Freshwater Alga

Although aquatic toxicity data are not available for products in the High Benzene Naphthas Category, there are sufficient read across data from constituent chemicals of those products and comparably complex products to fully characterize the toxicity of this category. Study specifics and robust summaries for analogous streams are available in the API Gasoline Blending Streams test plan on the US EPA HPV website. The use of data from selected read across materials to products in this category can be justified for the following reasons:

- Individual chemicals and complex products used for read across purposes contain a chemical class or combinations of chemical classes (i.e., olefins, aromatics, paraffins) that are found in streams from this category.
- Individual chemicals and complex products used for read across purposes have a carbon number or carbon number range that falls within the range of carbon numbers found in streams from this category.
- Individual chemicals and complex products used for read across purposes as well as the streams in this category are composed of chemicals that all act by a similar mode of toxic action.

The data in Appendix 6, Table A6-1 provides a comparison of the range of product compositions (i.e., carbon number, chemical class, weight percent) in the High Benzene Naphthas Category to products that have been used to characterize the aquatic toxicity of this category. This comparison illustrates the similarity in carbon number ranges between products in this category and the selected products with read across data.

The data in Appendix 6, Tables A6-2 (Fish), A6-3 (Daphnia), and A6-4 (Algae) establish the range of toxicity for products in this category, based on the read across data. Generally, the fish, invertebrate, and alga studies followed the OECD Guidelines 203, 202, and 201, respectively. For complex products, the test procedures used to develop the test material exposure solutions also applied the OECD guidance described in “Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures” (OECD, 1999). For these studies, the results are represented as lethal loading (LL) endpoints, a designation used to define results for multi-hydrocarbon mixtures, tested as water accommodated fractions [WAF], compared to the data developed for pure chemicals, which represent results as lethal concentration endpoints where test material is analytically verified. High benzene naphthas are likely to exhibit a moderate range of acute toxicity in freshwater fish and invertebrates and a moderate level of toxicity in freshwater algae.

For representative chemicals and products, experimental acute fish toxicity values range between 2.5 to 46.0 mg/L for two species (Table A6-2), while acute invertebrate (*Daphnia*) toxicity

values range between 0.9 to 32 mg/L for one species (Table A6-3). In comparison, alga toxicity values for one species range between 1.0 to 64 mg/L (for biomass or growth rate endpoints), while alga loading rate NOELR values range between 1.0 to 51 mg/L (for biomass and growth rate endpoints) (Table A6-4). Although not an HPV SIDS endpoint, chronic toxicity data from a representative high aromatic gasoline blending stream (API Gasoline Blending Streams Test Plan, 2003) gave similar results for fish and invertebrate toxicity:

Daphnia Reproductive EL50 = 14mg/L; NOEL <0.30mg/L
Fathead Minnow LL50 [survival] = 5.2mg/L;
NOEL[growth and survival] = 2.6mg/L

The fairly narrow range of effect is expected because the chemical constituents of products in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel and Opperhuizen, 1995), and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen, et al., 2000).

The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight (McCarty and MacKay, 1993; McCarty et al., 1991), supporting the assessment that these chemicals have equal potencies. When normalized to lipid content, the CBR is approximately 50 µmol of hydrocarbon/g of lipid for most organisms (Di Toro et al., 2000). Because the products in this category are all complex mixtures containing relatively similar series of homologous chemicals [paraffin, olefins and/or aromatic carbon number content within approximately C5-C11], their short-term toxicities are expected to fall within the range of toxicity demonstrated by the individual chemicals, as well as comparable products. The existing data are believed to form a sufficiently robust dataset to fully characterize the aquatic toxicity endpoints in the HPV Chemical Program for this category.

5.2 Assessment Summary for the Environment

The environmental impact of products in the High Benzene Naphthas Category has been determined by evaluating data developed for chemical components found in the products in this category and for similar complex products. The hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 0.9 - 65.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modelling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data shows that these products are likely to biodegrade significantly and have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates. Aquatic toxicity for products in this category can be predicted based on carbon number, measured or calculated toxicities of constituent hydrocarbons and constituent composition.

Extensive data on chemical components of the products in this category and on streams containing similar mixtures of complex hydrocarbons have demonstrated that, based on biological and physical degradation processes, products in the High Benzene Naphthas Category, although moderately toxic to aquatic species at exposure, are not expected to persist in the environment. The consistency of results in environmental studies for these materials justifies the designation of High Benzene Naphthas as a category for HPV.

6. PROGRAM SUMMARY AND RECOMMENDATIONS

The High Benzene Naphthas Test Plan has addressed petrochemical streams (products) derived from ethylene manufacturing processes. The category is comprised of 19 CAS numbers and 10 petrochemical streams. The category includes complex hydrocarbon mixtures containing primarily C5 through C11 olefins, paraffins, and aromatic molecules. The average benzene content of these streams is 55% but ranges from 10 –80%; toluene content ranges from 0.3 -40% depending on the stream. Virtually all of the benzene contained in the category streams is ultimately isolated as high purity benzene product, which is the primary use of the category streams. There are no known consumer uses for these category products. All of these products are produced and used on-site and/or transferred in closed systems so that occupational and public exposure to High Benzene Naphtha streams is very low.

Human Health Effects: Data on representative streams and read-across from chemical components indicate that High Benzene Naphtha streams are not acutely toxic by the oral, dermal or inhalation routes of exposure. It is unlikely that most streams in this category would cause significant genetic toxicity. Tested streams did not cause mutational events in bacteria, and a weak direct effect in mammalian cells from treatment with a C5-C10 fraction of Pyrolysis gasoline, was not confirmed *in vivo* by any expression of gene mutation in *Drosophila*. Although these streams contain substantial concentrations of benzene, a known clastogen, no cytogenetic damage was induced by oral treatment of rats with the Hydrogenated C6-C8 stream [55% benzene], demonstrating the inhibitory effects of other components in the stream, probably from competition for metabolic sites.

Benzene, as a predominant component in most streams is considered a key driver in establishing health effects within the SIDS battery of tests. To provide a conservative estimate of health hazard, results of benzene-induced systemic toxicity must be addressed – hazards from components should be considered hazards for the streams until sufficient data become available to show the specific combination of components does not present a hazard. However, as it has been demonstrated in the area of cytogenetics, the presence of biologically active components blended together can inhibit toxicity inducible by individual components. Limited repeat dose studies from representative streams in the High Benzene Naphthas Category demonstrated skin irritation and concomitant systemic effects from dermal exposure, and lethargy and labored respiration induced by inhalation at high doses. Results were similar to effects reported in the API Gasoline Blending Streams test plan (2003), effects from which animals recovered after 4 weeks without exposure. Such data suggest that toxicity of the blended streams may be less severe than that of individual components due to lower individual component concentrations, component interaction and competitive inhibition. No significant reproductive effects were reported in multigeneration studies of stream components. Developmental effects from components present in High Benzene Naphtha streams occurred primarily at doses that were maternally toxic as well. A developmental study in rabbits with a representative high benzene

naphtha stream did not result in adverse effects on any developmental parameters except for 1 high dose rabbit who aborted, and no malformations were induced.

Physicochemical, Environmental and Aquatic Endpoints: For environmental endpoints, measured data on components present in the products of the High Benzene Naphthas category, and on other complex products that contain a similar range of chemical classes and carbon numbers were used. Where measured data do not exist, calculated data for selected constituents of these naphthas have been developed using the EPIWIN© computer models described by EPA. The hydrocarbons that comprise this category have a very low potential to hydrolyze and do not photodegrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However, atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of representative constituent chemicals identified a range of 0.9 – 65.8 hours as a result of indirect hydrolysis by hydroxyl radical attack. Fugacity modeling demonstrated that members of this category partition primarily into the air, with slight partitioning into water and soil, and minimal partitioning into sediment. Read-across data shows that these products have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates but are likely to biodegrade significantly and are not expected to persist in the environment.

The extensive body of data available for mammalian and environmental endpoints on representative constituents of products in this category, on streams of similar complex hydrocarbon composition and some data from representative streams, are sufficient to fully characterize the potential toxicity for materials in this category and demonstrate the integrity of the category, itself. No additional testing is needed to meet the requirements of the HPV program.

New data on hydrocarbons present in High Benzene Naphtha streams that are developed in other HPV programs will be evaluated when available in the context of the present assessment. This category summary document will be amended should the new data result in substantial changes to the conclusions.

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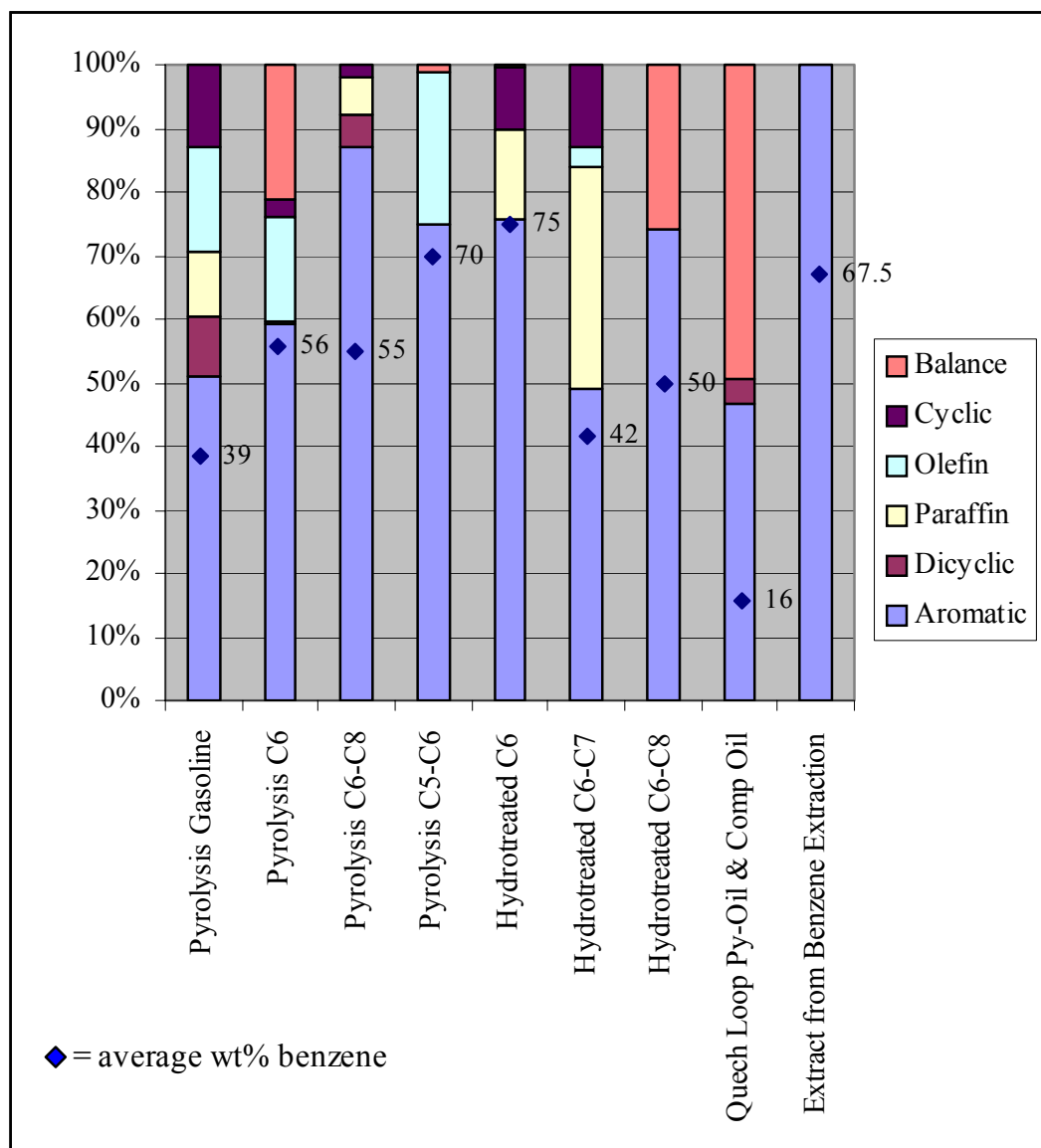
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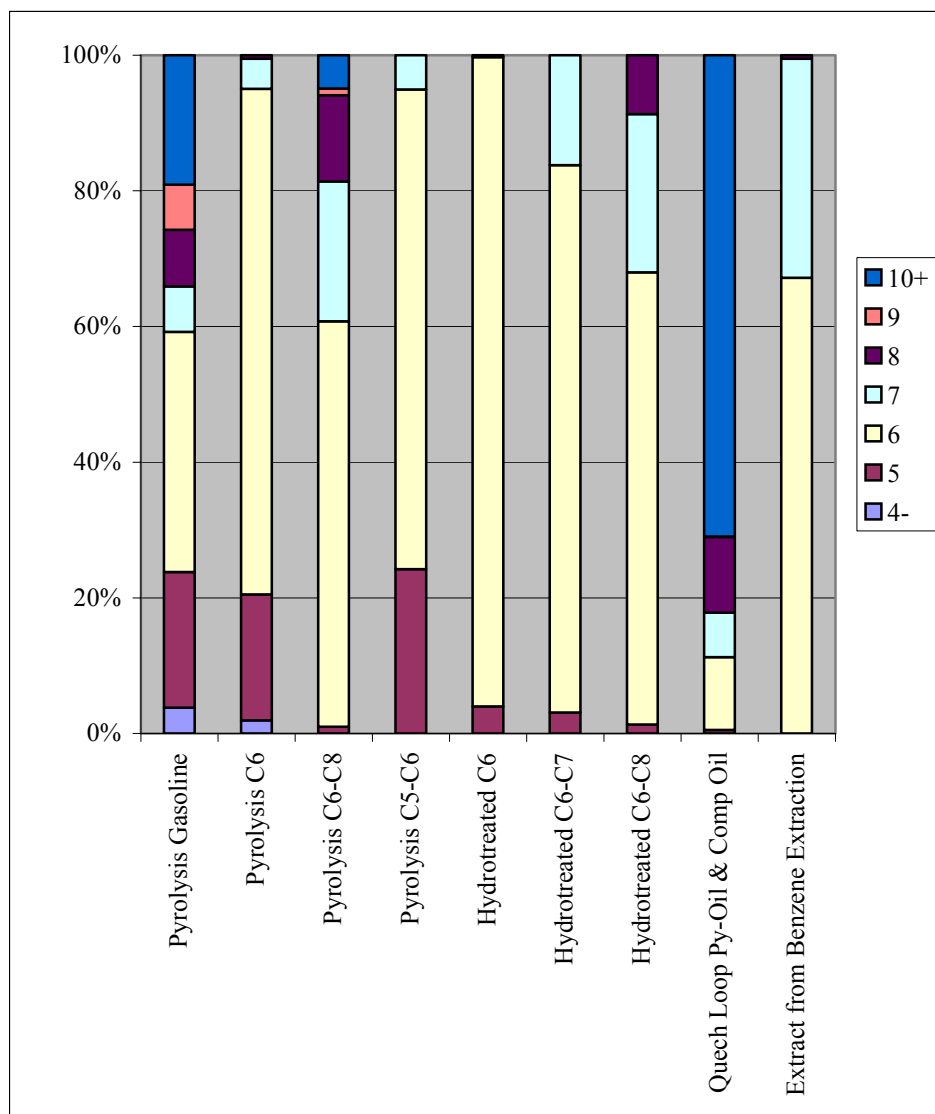
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Figure 4.
Stream Compositions: High Benzene Naphthas Category



Compositions are averages of the ranges reported for the complex, variable composition streams. In some cases, because of overlaps and variations in the way components were sometimes grouped in individual reports, the sum of the averages for the streams exceeded 100%. In those cases, compositions were normalized for plotting in Figure 4. When the total of the average of reported values was less than 100%, a “Balance” was added and included. Average wt% benzene content (actual average of reported values) of the streams is shown as diamonds with the average wt% given. Components grouped as “cyclic” include both paraffin and olefin cyclic hydrocarbons. The term “olefin” as used here does not include the cyclic olefins.

Figure 5
Stream Carbon Range Content - High Benzene Naphthas Category



Carbon range contents were normalized. Any apparent inconsistencies that may exist between Figure 4 and Figure 5 are largely due to normalization of the data.

Appendix 1: Ethylene Process Description

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as “steam cracking” or simply “cracking” and the furnaces are frequently referred to as “crackers.”

Subjecting the feedstocks to high temperatures results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker offgas. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primarily ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

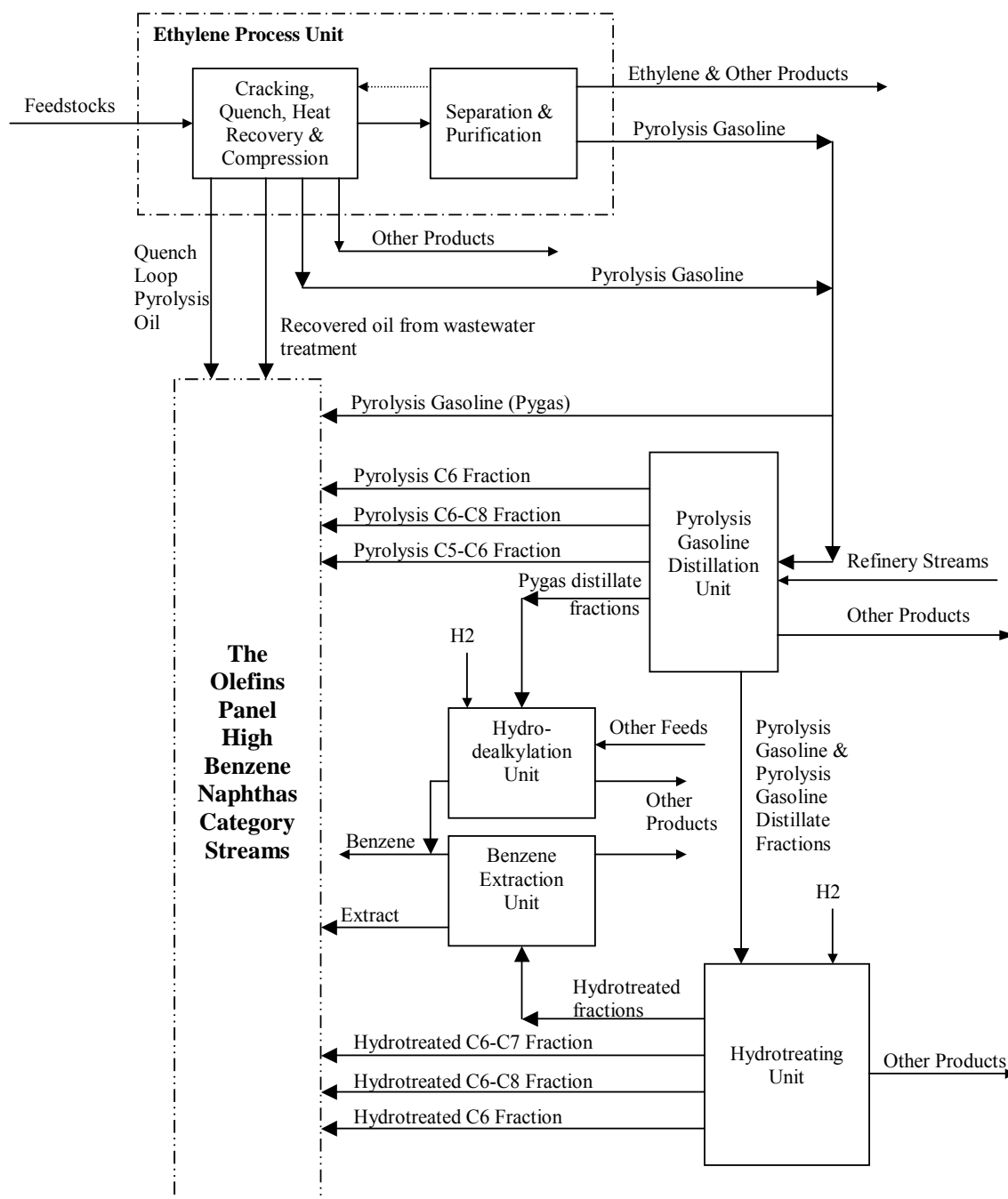
The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as “cracked gas” and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes,

a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges and in some cases further processed. It is a subset of these mixed streams that make up the constituents of the Low Benzene Naphthas Category.

The chemical process operations that are associated with the process streams in the Low Benzene Naphthas Category are shown in Figure 1.

Figure A1-1. Chemical Process Operations Associated with Process Streams in the High Benzene Naphthas Category.



Appendix 2: Composition**Table A2-1 Typical Stream Compositions (wt. %) for the High Benzene Naphthas Category.***(See notes 1-4 at the end of this table)*

Component Name	Pyrolysis Gasoline	Pyrolysis C6 fraction	Pyrolysis C6-C8 fraction	Pyrolysis C5-C6 fraction	Hydro-treated C6 fraction	Hydro-treated C6-C7 fraction	Hydro-treated C6-C8 fraction	Quench Loop Pyrol. Oil & Compressor Wash Oil	Recovered Oil from Waste Water treatment [see note 4]	Aromatic Extract from Benzene Extraction
Vinyl Acetate	9.9									
1,3-Butadiene	6.7	0.1-2.0								
C4's	0.5-5.0	0.1-1.5								
1,4-Pentadiene	0.3-0.9	0.1-2.0								
Isopentane (2-methylbutane)	2.0	0.1-1.0								
1-Pentene (Amylene)	0.6-4.0	1.0-3.0								
2-Methyl-1-Butene	1.0									
Pentene-2 (isomer mix)	0.2-1.8	0.1-5.0								
Isoprene (2-methylbutadiene-1,3)	0.6-10.0	2.0-6.0		6.0						
Pentenenes				10.0						
Pentane	10.0					1.0				
2-Methyl-2-Butene	1.2	2.0								
Other C5's	0.3						2.0			
3-methyl-1,2-butadiene		1.0-3.0								
1,3-Cyclopentadiene	1.0-20.0	0.1-5.0	1.0							
1,3-Pentadiene (isomer mix)	0.7-4.4	0.3-4.0								
Cyclopentene	0.6-5.0			8.0						
Cyclopentane	2.3				4.0	1.0-5.0				
1,5-Hexadiene	0.6									
2-Methylpentane	4.0				4.0					
2-Methyl-1-Pentene	0.0-2.2									
3-Methylpentane (Isohexane)	1.3				4.0	10.0-20.0				
Hexene-1	0.0-2.2									
Hexenes						2.0				
Methylcyclopentadiene	5.0		1.0							
Hexane Isomers			1.0-3.0			5.0-20.0				

Table A2-1 Typical Stream Compositions (wt. %) for the High Benzene Naphthas Category (cont).

Component Name	Pyrolysis Gasoline	Pyrolysis C6 fraction	Pyrolysis C6-C8 fraction	Pyrolysis C5-C6 fraction	Hydro-treated C6 fraction	Hydro-treated C6-C7 fraction	Hydro-treated C6-C8 fraction	Quench Loop Pyrol. Oil & Compressor Wash Oil	Recovered Oil from Waste Water treatment [see note 4]]	Aromatic Extract from Benzene Extraction
Hexane	0.0-9.0		1.0-5.0		6.0	2.0-15.0				
Methylcyclopentane	4.9					5.0-15.0				
1-Methylcyclopentene	0.1-2.4									
C6 non-aromatics		30.0						0.9		
Non-Aromatic hydrocarbons							20.0-26.0			
Benzene	15.0-62.0	35.0-77.0	30.0-80.0	70.0	75.0-75.7	40.0-69.0	40.0-60.0	10.0-21.6		60.0-75.0
1,3-Cyclohexadiene	0.5-2.0									
Cyclohexane	2.0				6.0	1.0-3.0				
Cyclohexene	0.6									
Cyclohexadienes	0.1-2.3									
3-Ethylpentene-1		1.0								
C6 olefin	0.2-1.9									
Heptenes						2.0				
2-Methylhexane						2.0				
Heptane Isomers						1.0-5.0				
Heptane	0.4-2.0		1.0			1.0-5.0				
C7 Paraffins & Naphthenes	0.3-1.1									
C7 Olefins	0.0-1.2									
Methylcyclohexane						1.0-3.0				
C7 Non-aromatics		3.0						2.2		
Toluene	17.4	0.5-5.0	15.0-25.0	5.0	0.3	3.0-15.0	10.0-25.0	5.0-10.9		25.0-40.0
4-Vinylcyclohexene [Butadiene dimer]	0.1-1.0									
C8 Nonaromatics								1.3		
Ethylbenzene	0.3-5.5	1.0	1.0-3.0					1.0-3.0		
C8 Aromatics							3.0-10.0			1.0
Xylenes, mixed	10.0		1.0-10.0					1.5		
Styrene	10.0		1.0-10.0					10.0-15.0		
C9 Aromatics	0.4-1.7									

Table A2-1 Typical Stream Compositions (wt. %) for the High Benzene Naphthas Category. (cont.)

Component Name	Pyrolysis Gasoline	Pyrolysis C6 fraction	Pyrolysis C6-C8 fraction	Pyrolysis C5-C6 fraction	Hydro-treated C6 fraction	Hydro-treated C6-C7 fraction	Hydro-treated C6-C8 fraction	Quench Loop Pyrol. Oil & Compressor Wash Oil	Recovered Oil from Waste Water treatment [see note 4]]	Aromatic Extract from Benzene Extraction
Ethyltoluenes	0.1-2.0									
C9 Paraffins & Naphthenes	0.3-1.3									
1,3,5-Trimethylbenzene (mesitylene)	3.0									
C10+								40.6		
1,2,4-Trimethylbenzene (Pseudocumene)	0.0-3.3		1.0							
4-Methylstyrene	0.0-3.3									
Cyclopentadiene/ Methylcyclopentadiene Codimers	0.9-4.4		1.0-3.0							
Dicyclopentadiene	20.0		1.0-5.0					3.7		
1-Decene	1.5									
Vinyl Toluene	0.1-1.1									
Dihydro-dicyclopentadiene	2.0									
Decane	0.1-5.0									
C10 Aromatics	1.6									
C10's								1.6-27.0		
Indene	0.6-5.0									
C11+								38.8-50.0		
Naphthalene	15.0							4.3-10.0		
Methylnaphthalene	2.9									
1-Methylnaphthalene	1.0									
1,1''-Biphenyl	0.1-0.9									
C10 Olefins	1.2									

Note 1: The composition data shown above are composites of reported values..

Note 2: The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.

Note 3: The listed highs and lows should not be considered absolute values for these limits. They are instead highs and lows of reported values.

Note 4: No specific composition data are available. This stream is expected to contain components of Pyrolysis Gasoline

Appendix 3.

Summary Results from Existing Human Health Effects Data for Chemical Components and Streams of High Benzene Naphthas Category

(Note: This table is the product of a good faith effort to briefly summarize results of toxicity studies that were available to the reviewer for SIDS endpoints. Results from non-SIDS endpoints are not included. Since all information for a particular chemical may not have been available to the reviewer, the results presented should not be considered as final assessments of the hazards of the listed chemicals. Component data were not reviewed for data adequacy. Robust summaries for the listed components will not be submitted with the Test Plan.)

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Vinyl Acetate	Oral LD50 = 2.9 g/kg; inhalation LC50 = 3680 ppm [4h]	Negative in Ames Test	Positive in mouse bone marrow micronucleus test by i.p. but negative in rats and mice by inhalation and oral; positive in in-vitro chrom ab	4 and 13-wk rat and mouse inhalation study: decrease in BW gain, respiratory tract effects; no clearly treatment related effects in 4 and 13-wk rat and mouse oral	In rat inhalation study, no embryolethality or teratogenicity seen; fetal growth retardation seen at maternally toxic doses. In rat oral study, no effects.	In an oral rat 2-gen repro study, no effects were seen except for reduction in BW gain in high-dose F1 pups.		Review: IRIS ⁸ – 1990; HSDB ⁹ ; ATSDR – 1992 ⁴
1,3-Butadiene	Rat inhalation LC50[4h] = 129,000 ppm	Negative in UDS in mouse and rat, Drosophila; negative and positive in mouse lymphoma; positive in Ames, CHO and in vivo mouse spleenocyte HPRT tests and mouse spot test	Positive in mouse dominant lethal but negative in rat; positive in mouse bone marrow micronucleus and chrom. ab.; negative in rat bone marrow micronucleus	Many studies: Toxicity to blood cells in mice; no effects in rats [inhalation]	Effects seen at maternally toxic doses	Will become available through OECD SIDS	Olefins Panel's Crude Butadiene C4 Category, OECD SIDS	Reviews: ECETOC Special Report No. 12 - 1997 ¹⁰ ; ATSDR ¹¹ - 1993

⁸ IRIS: EPA Integrated Risk Information System

⁹ HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc.]

¹⁰ ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Isoprene (2-methylbutadiene-1,3)	Rat oral LD50= 2.1 g/kg; inhalation LC50 [4h] = 64,500 ppm	Negative in Ames Test	Negative in in-vitro CHO chrom. ab., mouse bone marrow chrom. ab. and rat lung cell micronucleus [inhalation]; positive in mouse bone marrow micronucleus [inhalation]	Many studies: Effect on testes in rats seen at 26 wks but not at 13 wks; effects on blood cells, nasal epithelium, liver, stomach, and testes in mice [inhalation]	No effects in rats; fetotoxicity in mice	Limited repro tox data [sperm motility, vaginal cytology, histopath of repro organs]obtained as part of 13-wk inhalation study: [slight effect on testis in rats; effects on testes, epididymus, sperm, estrus cycle in mice]	Olefins Panel's C5 Non-Cyclics Category/ICCA	Review: IARC ¹² - 1999
Pentenenes				2-pentene: 4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 2 g/kg/day w/60% mortality			International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; also, pentenes are likely to have a toxicity profile similar to hexenes which will be addressed by the Higher Olefins Panel	Halder et al., 1985

¹¹ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

¹² IARC: International Agency for Research on Cancer

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Pentane	Rat oral: LD50>2 g/kg; inhalation LC50[4h] >7000 ppm	Negative in Ames Test	Negative in rat bone marrow micronucleus [inhalation] and dominant lethal [i.p.]; positive [not reproducible] in in-vitro CHO chrom.ab.	90-day rat inhalation: no effect at ~ 7000ppm. 16 wk and 7-30 wk rat inhalation neurotox evaluations : negative With 50/50 blend of n-butane and n-pentane, in a 90-day rat inhalation study with scope limited to evaluation of nephrotoxicity: decrease in BW and male hydrocarbon nephropathy.	No effect in rat oral	No effect on repro organs in 90-day rat inhalation	API [addressed in Petroleum Gases Test Plan]; International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; OECD SIDS	Review: McKee et al., 1998; Galvin and Marashi, 1999
1,3-Cyclopentadiene	Rat oral: 4/5 died at 1 g/kg; inhalation LC50 [4h] = 39 mg/L			Mild liver and kidney effects in rats after 35 exp. of 500 ppm ; no effects in guinea pigs, rabbits, dogs after 135 exp. of 250 ppm, or in dogs after 39 additional exp of 400 ppm and 16 additional exp of 800 ppm [inhalation]				ACGIH ¹³ , RTECS ¹⁴ , EPA Documents [86960000024, 86960000121S
Cyclopentene	Rat oral LD50 = 1.66 g/kg; inhalation LCLo [4h] = 16,000 ppm							RTECS

¹³ ACGIH: American Conference of Governmental Industrial Hygienists

¹⁴ RTECS: Registry of Toxic Effects of Chemical Substances

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
3-methylpentane (Isohexane)				16 wk and 7-30 wk rat inhalation neurotox evaluations : negative				Frontali et al., 1981
Hexane isomers [Commercial Hexane tested: 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane]		Negative in Ames Test, CHO HPRT	Negative in in-vitro CHO chrom. ab. and rat bone marrow chrom. ab. [inhalation]	No neurotoxicity; male rat hydrocarbon nephropathy [inhalation]	No effects in rats via inhalation	No effect in rat 2-gen study via inhalation except decrease in weight gain in high dose offspring		Daughtrey et al., 1994 a,b; 1999; Kirwin et al., 1991
Hexane	Rat oral LD50=28.7 g/kg; inhalation LC50[4h] = 48,000 ppm	Negative in Ames Test and in vitro UDS	Negative in in-vitro CHO chrom. ab. , inhalation dominant lethal and mouse micronucleus [inhalation and IP]; positive in rat oral bone marrow chrom. ab.	Several studies: Effects on peripheral nervous system and testes	Negative in inhalation and oral developmental studies	No repro tox studies found; testicular atrophy seen in subchronic inhalation studies	OECD SIDS - ICCA	Review: ATSDR ¹⁵ – 1999; rat chrom. ab. report in HSDB ¹⁶
Methylcyclopentane				4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 0.5 g/kg/day but lesions at 2g/kg w/40% mortality				Halder et al., 1985

¹⁵ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

¹⁶ HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc]

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Benzene	Rat oral LD50=810 mg/kg; Rat oral LD50=1000mg/kg [Smyth et al., 1962] Inhalation LC50 [4h] = 13,700 ppm	Negative in Ames Test, mouse lymphoma, CHO HPRT, in-vitro UDS, Drosophila; positive in mouse spleen HPRT	Positive in vitro/in vivo in numerous studies and species [oral, inhalation]: in-vitro human lymphocytes; chrom. ab. and micronucleus in mouse bone marrow and spleen lymphocytes; rat bone marrow chrom. ab. and micronucleus	Many studies: Primary effect toxicity to blood cells	Several studies: fetotoxic at maternally toxic doses; not tetratogenic	No standard repro studies; most inhalation studies with repro parameters indicate no effect on reproductive indices, even at high doses	OECD SIDS	Review: ATSDR – 1997; EU Risk Assessment – 2001 [Draft]
Cyclohexane	Rat oral LD50 > 5 g/kg; inhalation LC50[4h] = 4044 ppm	Negative in Ames Test, mouse lymphoma, human lymphocyte UDS	Negative in rat bone marrow chrom. ab. [inhalation]	Effects on liver in mice and rats; on liver and kidney in rabbits [inhalation]	No effects seen in rats or rabbits [inhalation]	No effects in rat 2-gen inhalationrepro at doses not maternally toxic	OECD SIDS	Review: SRC Technical Support Document #TR-86-030 [Beals et al., 1986, draft] ¹⁷ ; EU Risk Assessment – 2000 [Draft] Bamberger, 1996; Kreckman, 1997; Malley, 1996 a,b

¹⁷ SRC: Syracuse Research Corporation Center for Chemical Hazard Assessment, prepared for Test Rules Development Branch, Existing Chemical Assessment Division, Office of Toxic Substances

Smyth, H.F. Carpenter, C.P., Weil, C.S. et al., 1962. Range-finding toxicity data. List VI. Ind. Hyg. J 23: 95-107.

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Toluene	Rat oral LD50 = 5.5 – 7.53 g/kg; inhalation LC50[4h] = 8000 - 8800 ppm	Negative in Ames Test, SHE transformation, and Drosophila SLRL; equivocal in mouse lymphoma	Negative in in-vitro human lymphocyte and CHO chrom. ab. dominant lethal [oral], chrom. ab. in mice [oral] and rats [inhalation], and mouse micronucleus [oral]	Many studies: Effects on central nervous system; hearing loss in rats	In rats and mice: lower birth weight, delayed postnatal development and behavioral effects [inhalation]	No effects in mouse 2-gen inhalation repro study; in rats, effect on sperm count and epididymal weight at 2000 ppm, but no effect on fertility	OECD SIDS	Review: ATSDR ¹⁸ – 2000; IARC ¹⁹ – 1999; EU Risk Assessment - 2001 Genetic toxicity review: McGregor, 1994.
Ethylbenzene	Rat oral LD50> 3.5 g/kg; inhalation LC50[4h] LC50 = 4000 ppm	Negative in Ames Test, Drosophila SLRL, and in-vivo UDS in mouse hepatocytes; equivocal in mouse lymphoma	Negative in in-vitro CHO and RL4 cells chrom. ab. and in inhalation/i.p. mouse micronucleus	Several studies: Effects seen in liver, kidney, and lung in rats and mice; hearing loss in rats via inhalation	No effects in rabbits; only supernumerary ribs seen in rats	No repro study; in subchronic rat and mouse studies, no effects seen in gonads sperm, extrus cycle	OECD SIDS	Review: ATSDR ²⁰ - 1999
Xylenes, mixed	Rat oral LD50 = 3.5-8.6 g/kg; Rat inhalation [4h] LC50 = 6,350 - 6,700 ppm	Negative Ames Test and mouse lymphoma	Negative in human lymphocytes [only w/o S9 tested] and CHO chrom. ab.	Many studies: liver, and nervous system effects via inhalation; hearing loss in rats via inhalation; nervous system effects via oral exposure	Fetotoxic effects seen in rat and mouse [oral, inhalation], mostly secondary to maternal toxicity	Negative in rat repro [exposed by inhalation 131 days prior to mating, during mating, gestation, day 5-20 of lactation]; no effect on repro organs in rat and mouse	ACC Toluene Xylene Panel/OECD SIDS/ICCA	Review: ATSDR – 1995; WHO EHC - 1997 ²¹ ; ECETOC - 1986

¹⁸ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

¹⁹ IARC: International Agency for Research on Cancer

²⁰ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

²¹ WHO EHC: World Health Organization, International Programme on Chemical Safety. Environmental Health Criteria

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Styrene	Rat oral LD50 \geq 5 g/kg; inhalation LC50 [4h] = 4940 ppm	Inconsistent results in Ames Test	Inconsistent results in in-vitro chrom. ab. tests; negative in chrom. ab. and micronucleus tests in mice and rats by oral and inhalation exposure	Many studies: Effects on liver in rats [oral, inhalation] and mice [inhalation]; hearing loss in rats [inhalation]; respiratory tract in rats [inhalation]; lungs in mice [oral]	No birth defects in rats [oral, inhalation] or in mice, rabbits and hamsters [inhalation]; other effects seen only at maternally toxic doses	Negative in rat 3 gen repro study [oral]	OECD SIDS	Reviews: ATSDR – 1992; IARC ²² – 1994 Brown, 1991, 1993 [repro/devel]
Dicyclopentadiene	Rat oral LD50 ranged from 347 – 820 mg/kg; inhalation LC50[4h] ranged from 359 to 500-1000 ppm	Negative in Ames Test	Negative in in-vitro CHO and CHL chrom. ab.	Many studies: Most studies showed no effects in rats or mice in dietary or inhalation studies except male rat hydrocarbon nephropathy in inhalation studies	No effect in rats in oral [diet] studies	Effects only at maternally toxic doses in rat 3-gen repro study [in diet]	OECD SIDS	Review: ECETOC ²³ – 1991 JETOC ²⁴ Issue 3 No. 32, 1998 [CHL chrom. ab and OECD 422 studies]; NTP ²⁵ [CHO chrom. ab.]

²² IARC: International Agency for Research on Cancer

²³ ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

²⁴ JETOC: Japanese Chemical Industry Ecology – Toxicology and Information Center

²⁵ NTP: National Toxicology Program – personal communication

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Naphthalene	Rat oral LD50 ranged from 2200 to 2600 mg/kg; no effect at 78 ppm [4h] inhalation	Negative in Ames Test, transformation, in-vivo UDS in rat liver	Negative in mouse micronucleus; positive in in-vitro CHO chrom. ab.	Many studies: Toxicity to blood cells in dogs [hemolytic anemia][oral]but not rats or mice; cataracts in rabbits, rats, mice, guinea pigs [oral]; local irritative effects after inhalation in rats and mice	No birth defects in rabbits, rats, and mice [oral]; reduced litter size in mice at maternally toxic doses [oral on gestation day 7-14]; no effect in rabbits exposed orally on gestation days 6-18		OECD SIDS	Reviews: ATSDR ²⁶ – 1995; EU Risk Assessment Document – Draft 2001

²⁶ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

HPV CHEMICAL CATEGORY SUMMARY: HIGH BENZENE NAPHTHAS

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
STREAMS								
Rerun Tower Overheads [approx. 40% benzene, 13% toluene, 26% C5, 20% other] [C5-10 Fraction of Pyrolysis Gasoline HPV stream]	Rat oral LD50 > 2 g/kg; rabbit dermal LD50>2g/kg	Negative Ames Test, Drosophila (point mutation), and transformation (BALB-c/3T3 and C3H 10T½); weakly positive in mouse lymphoma and bacterial DNA repair	Negative in Drosophila chromosome loss and chromosome aberration studies	Rabbit 21-day dermal irritation: NOAEL (systemic) = 1.0 ml/kg/day (top dose); NOAEL (irritation) = <0.10 ml/kg/day	No effects in rabbits in oral teratology pilot and main studies			Robust Summaries
Dripolene [HPV stream: Pyrolysis Gasoline]	Rat oral and dermal LD50 > 2 g/kg							Robust Summary
Hydrogenated Pyrolysis Gasoline [55% benzene, 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 2% hexane, 3% cyclohexane] [HPV stream: Hydrotreated C6-8 Fraction]	Rat Oral LD50 = 5.17 g/kg; inhalation 4h LC50>12,408 ppm	Negative in Ames Test, in-vitro UDS; positive in transformation	Negative in micronucleus [mouse oral]	Rat 5 day inhalation: NOAEL <4869 ppm [deaths, bodyweight]				Robust Summaries

Appendix 4.

Sources of Data for Hazard Evaluations for Mammalian Toxicity

[All streams are subject to the OSHA Benzene Standard. For hazard communication, the final hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.]

STREAM	SOURCES OF DATA FOR HAZARD EVALUATION [These data will be evaluated using scientific judgment and complying with the requirements of the OSHA benzene, 1,3-butadiene, and hazard communication standards]
Pyrolysis Gasoline	<ul style="list-style-type: none"> • Available data for components [benzene, 1,3-butadiene, cyclohexane, cyclopentadiene, cyclopentene, 3-methylpentane, dicyclopentadiene, ethylbenzene, hexane, isoprene, methylcyclopentane, naphthalene, pentadiene, pentane, pentenes, styrene, toluene, vinyl acetate, xylene] • Data for streams containing Pyrolysis Gasoline or fractions thereof [Pyrolysis Gasoline Fractions, Dripolene, Hydrogenated Pyrolysis Gasoline (robust summaries provided)] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics and Resin Oils and Cyclodiene Dimer Concentrates categories] • Data for gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Data for hexenes being developed by the ACC Higher Olefins Panel, for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category, and for pentane which is addressed in the API Petroleum Gases Test Plan • Literature data regarding interactions between components present in these streams
Pyrolysis C6 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, 1,3-butadiene, cyclopentadiene, ethylbenzene, isoprene, pentenes, pentadiene, toluene] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics Category] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes), for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category • Literature data regarding interactions between components present in these streams

STREAM	SOURCES OF DATA FOR HAZARD EVALUATION [These data will be evaluated using scientific judgment and complying with the requirements of the OSHA benzene, 1,3-butadiene, and hazard communication standards]
Pyrolysis C6-C8 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, dicyclopentadiene, ethylbenzene, hexane, styrene, toluene, xylene] • Literature data regarding interactions between components present in these streams
Pyrolysis C5-C6 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, cyclopentene, isoprene, pentenes, toluene] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes) • Literature data regarding interactions between components present in these streams
Hydrotreated C6 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, cyclohexane, hexane, 3-methylpentane] • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Literature data regarding interactions between components present in these streams
Hydrotreated C6-C8 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, toluene and other identified components] • Data for Hydrogenated Pyrolysis Gasoline (robust summaries provided) • Literature data regarding interactions between components present in these streams
Quench Loop Pyrolysis Oil and Compressor Oil	<ul style="list-style-type: none"> • Available data for components [benzene, dicyclopentadiene, ethylbenzene, naphthalene, styrene, toluene, xylene and other identified components] • Literature data regarding interactions between components present in these streams
Recovered Oil from Waste Water Treatment	<ul style="list-style-type: none"> • Available data for components, on a case-by-case basis
Aromatic Extract from Benzene Extraction Unit	<ul style="list-style-type: none"> • Available data for components [benzene, toluene] • Literature data regarding interactions between components present in these streams

Appendix 5. Biodegradation

Table A5-1.

Read Across Data used to Characterize the Biodegradability of the High Benzene Naphthas Category from Chemicals Contained by Products in this Category and Chemically Complex Products not in this Category, but that Contain Like-Chemicals.

CHEMICAL / PRODUCT	CARBON NUMBER	PERCENT BIODEGRADATION ^a (28 days)	REFERENCE
n-Pentane	5	87	IHSC ^e
Isopentane	5	71	IHSC ^e
Cyclohexane	6	77	IHSC ^e
Alkenes, C6 Rich	6 ^b	21	HOP ^f
1-Hexene (linear)	6	67-98 ^c	^g
Benzene	6	63	Robust Summary Provided with this test plan
Alkenes, C7-C9, C8 Rich	7-9	29	HOP ^f
p-Xylene	8	89	XIC ^h
Styrene	8	100 (14 days) ^c	ⁱ
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42 ^d	API ^j
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74 ^d	API ^j
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-9	96 ^d	API ^j
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9 ^b	78	IHSC ^e
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^b	61	IHSC ^e

a OECD 301F, manometric respirometry test

b Predominant carbon number or range

c BOD test

d Test method for determining the inherent aerobic biodegradability of oil products and modification of ISO/DIS 14593

e Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)

f Robust summary from the Higher Olefins Panel: C6, C7, C8, C9, and C12 Internal Olefins and C16 and C18 Alpha Olefins Category Test Plan (submitted)

g These chemicals are in the OECD SIDS program (Chemicals Inspection & Testing Institute, Japan 1992)

h Robust summary submitted with High Benzene Naphthas test plan

i Part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16

j Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table A5-2

Composition (Weight Percent) of Three Gasoline Streams with Biodegradation Data Used to Read Across to Products in the High Benzene Naphthas Category.

Naphtha, (Pet.) Light Alkylate		Naphtha, (Pet.) Light Catalytically Cracked		Naphtha, (Pet.) Light Catalytically Reformed	
CAS# 64741-66-8	Weight %	CAS# 64741-55-5	Weight %	CAS# 64741-63-5	Weight %
Isopentane	12.61	n-hexane	1.69	n-heptane	3.59
2,3 dimethyl butane	4.74	n-pentane	1.71	n-hexane	4.69
2,4 dimethyl pentane	4.09	isopentane	4.7	n-pentane	8.05
2,3 dimethyl pentane	2.25	2,3 dimethyl pentane	1.12	Isopentane	11.39
2,2,4 trimethyl pentane	23.92	2 methyl hexane	1.58	2,2 dimethyl butane	1.26
2,2,3 trimethyl pentane	1.76	3 methyl hexane	1.45	2,3 dimethyl butane	1.11
2,3,3 trimethyl pentane	8.99	2 methyl pentane	3.64	2,3 dimethyl pentane	1.70
2,3,4 trimethyl pentane	11.56	3 methyl pentane	2.20	2 methyl hexane	4.30
2,3,5 trimethyl hexane	1.25	methyl cyclopentane	1.87	3 methyl hexane	5.18
2,5 dimethyl hexane	4.34	methyl cyclohexane	1.19	2 methyl pentane	5.17
2,4 dimethyl hexane	3.60	1-pentene	1.25	3 methyl pentane	4.00
2,3 dimethyl hexane	2.60	2-methyl-1-butene	2.31	benzene	8.37
1methyl-1ethyl cyclopentane	9.44	2-methyl-2-butene	5.35	toluene	29.77
		trans-2-pentene	3.33		
		cis-2-pentene	1.94		
		2-methyl-1-pentene	2.31		
		cis-3-hexene	1.67		
		trans-2-hexene	1.97		
		2-methyl-2-pentene	1.83		
		1-methyl cyclopentene	1.85		
		ethylbenzene	1.47		
		m-xylene	3.05		
		p-xylene	1.34		
		o-xylene	1.83		
		benzene	1.48		
		toluene	6.73		

Appendix 6. Aquatic Toxicity

Table A6-1

Approximate Weight Percent and Carbon Number Comparison of Hydrocarbons in High Benzene Naphthas Category and Comparable Products^a.

Substance Name	Olefins		Aromatics		Paraffins	
	% (wt.)	C # ^b	% (wt.)	C # ^b	% (wt.)	C # ^b
Products in High Benzene Naphtha Category	1-34	5-9	>40-100	6-11	>4-75	5-10
Alkenes, C6 Rich	100	5-7	0	-	0	-
Alkenes, C7-9, C8 Rich	100	7-9	0	-	0	-
C8-C10 Aromatics, Predominantly C9 Aromatics	0	-	>97	8-10	<3	-
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	0	-	>94	10-14	<6	-
Naphtha (petroleum), Light Alkylate (gasoline stream)	0	-	0	-	92	5-8
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	24	5-6	16	6-8	21	5-7
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	0	-	38	6-7	50	5-7

a Approximate weight percent and carbon number ranges of the predominant chemical components by chemical class [olefins/aromatics/paraffins] for selected products contained by this category and for comparable products not in this category that have aquatic toxicity data that can be used as read across data for this category; % compositions may not total 100%.

b Predominant carbon number range

Table A6-2

Acute Fish Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the High Benzene Naphthas Category

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY ^a (96-hr, mg/L)	REFERENCE
n-Pentane	5	<i>Oncorhynchus mykiss</i>	LC50 = 4.3	IHSC ^d
n-Hexane	6	<i>Pimephales promelas</i>	LC50 = 2.5	IHSC ^d
Benzene	6	<i>Oncorhynchus mykiss</i>	LC50 = 5.9	^e
Alkenes, C6 Rich	5-7 ^b	<i>Oncorhynchus mykiss</i>	LL50 = 12.8	HOP ^f
Mixed Cycloparaffins, C7-8, C7 Rich	7	<i>Oncorhynchus mykiss</i>	LC50 = 5.4 ^c	IHSC ^d
Toluene	7	<i>Pimephales promelas</i>	LC50 = 14.6	IHSC ^d
Alkenes, C7-9, C8 Rich	7-9 ^b	<i>Oncorhynchus mykiss</i>	LL50 = 8.9	HOP ^f
o-Xylene	8	<i>Pimephales promelas</i>	LC50 = 16.4	XIC ^g
p-Xylene	8	<i>Oncorhynchus mykiss</i>	LC50 = 2.6	XIC ^g
p-Xylene	8	<i>Pimephales promelas</i>	LC50 = 8.9	XIC ^g
Ethylbenzene	8	<i>Pimephales promelas</i>	LC50 = 12.1	^h
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 ^b	<i>Pimephales promelas</i>	LL50 = 8.2	API ⁱ
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8 ^b	<i>Pimephales promelas</i>	LL50 = 46	API ⁱ
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	5-7 ^b	<i>Pimephales promelas</i>	LL50 = 34	API ⁱ
1,2,4-Trimethyl-benzene	9	<i>Pimephales promelas</i>	LC50 = 7.7	IHSC ^d
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 ^b	<i>Oncorhynchus mykiss</i>	LL50 = 18.0	IHSC ^d
C8-C14 Aromatics, Predominantly alkyl Naphthalenes and Naphthalene	10-12 ^b	<i>Oncorhynchus mykiss</i>	LL50 = 3.0	IHSC ^d

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; values cited as “concentration” are based on measured values

b Predominant carbon number or range

c 93-hour value

d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)

e Galassi, S., M. Mingazzini, L. Viagano, D. Cesareo, and M.L. Tosato, 1988. Benzene is in the OECD SIDS program

f Robust summary from the Higher Olefins Panel HPV Test Plan (submitted)

g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16

h Ethylbenzene is in the OECD program and was reviewed as part of SIAM 15

i Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted)

Table A6-3

**Acute Invertebrate Toxicity Data for Selected Chemicals and Complex Products
used to Characterize the Toxicity of Products in the High Benzene Naphthas Category.**

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY ^a (48-hr, mg/L)	REFERENCE
n-Pentane	5	<i>Daphnia magna</i>	EC50 = 2.7	IHSC ^e
n-Hexane	6	<i>Daphnia magna</i>	EC50 = 2.1	IHSC ^e
Cyclohexane	6	<i>Daphnia magna</i>	EC50 = 0.9	IHSC ^e
Benzene	6	<i>Daphnia magna</i>	EC50 = 18 ^b	^f
Toluene	7	<i>Daphnia magna</i>	EC50 = 14.9	Hermens et al ^j
o-Xylene	8	<i>Daphnia magna</i>	EC50 = 1.0	XIC ^g
m-Xylene	8	<i>Daphnia magna</i>	EC50 = 4.7	XIC ^g
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7 ^c	<i>Daphnia magna</i>	EL50 = 10	API ^h
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 ^c	<i>Daphnia magna</i>	EL50 = 32	API ^h
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 ^c	<i>Daphnia magna</i>	EL50 = 18	API ^h
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 ^c	<i>Daphnia magna</i>	EL50 = 21.3	IHSC ^e
Naphthalene	10	<i>Daphnia magna</i>	EL50 = 16.7 ^d	ⁱ
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^c	<i>Daphnia magna</i>	EL50 = 3.0	IHSC ^e

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; values cited as “concentration” are based on measured values

b 24-hour study

c Predominant carbon number or range

d Based on nominal values

e Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)

f Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)

g Xylenes are part of the Xylene ICCA Consortium and were reviewed by OECD at SIAM 16

h Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)

i Naphthalene is part of the OECD program and was reviewed in SIAM 13

j Hermens, J., Canton, H., Janssen, P., and deJong, R. (1984). Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anesthetic potency: acute lethal and sublethal toxicity to *Daphnia magna*. *Aquat Toxicol* 5: 143 –154. In EU Toluene SIAR 10888

Table A6-4

Alga Toxicity Data for Selected Chemicals and Complex Products Used to Characterize the Toxicity of Products in the High Benzene Naphthas Category

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY^a (72-hr, mg/L)	REFERENCE
n-Pentane	5	<i>Pseudokirchneriella subcapitata</i> ^b	EbC50 = 10.7 ErC50 = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC ^d
Benzene	6	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 29	^e
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7 ^c	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 8.5 NOELRb = 5.0	API ^f
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8 ^c	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 45 NOELRb = 18	API ^f
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 ^c	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 64 NOELRb = 51	API ^f
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 ^c	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 2.6 ErL50 = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHSC ^d
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^c	<i>Pseudokirchneriella subcapitata</i>	EbL50 = 1-3 ErL50 = 1-3 NOELRb = 1.0 NOELRr = 1.0	IHSC ^d

- a Endpoint is growth inhibition; EbC = Effect Concentration for biomass; ErC = Effect Concentration for growth rate; EbL = Effect Loading for biomass; ErL = Effect Loading for growth rate; NOECb = No Observed Effect Concentration for biomass; NOECr = No Observed Effect Concentration for growth rate; NOELRb = No Observed Effect Loading Rate for biomass; NOELRr = No Observed Effect Loading Rate for growth rate; values cited as “concentration” are based on measured values
- b Formally known as *Selenastrum capricornutum*
- c Predominant carbon number or range
- d Covered by the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (expected to be submitted at SIAM 19)
- e Benzene is in the OECD program and was reviewed as part of SIAM 15 (Galassi, et. al., 1988)
- f Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (2003)

Appendix 7.

American Chemistry Council

Olefins Panel Sponsored HPV Test Categories.

Category Number	Category Description
1	Crude Butadiene C4
2	Low Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (C3) - Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7, 8, & 9	Resin Oil & Cyclodiene Dimer Concentrates
10	Fuel Oils
11	Pyrolysis C3+ and Pyrolysis C4+

Attachments [Separate documents]

Attachment 1a. Robust Summaries: PhysicoChemical and Environmental Fate

Attachment 1b. Robust Summary: Biodegradation Study Benzene

Attachment 1c. Robust Summaries: Mammalian Toxicology